Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

May 10, 2016

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Pleiades Supercomputer Augmented with New Broadwell Processors

- The HECC Supercomputing Systems team augmented the Pleiades supercomputer with 14 of the latest-generation Intel E5-2680v4 (Broadwell) compute racks, expanding the system's capability and increasing its total peak performance from 5.34 to 6.28 petaflops.
- HECC engineers integrated the racks into the Pleiades InfiniBand fabric using their in-house live-integration method to minimize the impact on users for production computing cycles.
- In order to accommodate the Broadwell racks, 16 Westmere racks were removed from Pleiades to provide the power required for the new equipment.
- The system was delivered in two shipments; 10 racks arrived for the initial deployment, followed by another four racks a few weeks later.
- In the second of two test phases, all users were given early access to the Broadwell nodes, without charge, for testing the new hardware with their codes (see slide 4).

Mission Impact: To meet NASA's requirements for high-performance computing, HECC must regularly and significantly upgrade and replace the supercomputing resources provided to the agency.

The installation of new Intel "Broadwell" nodes on the Pleiades supercomputer provides users with about four times the performance of the baseline Westmere nodes. The augmentation increased the system's peak performance by nearly 18 percent.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, CSC Government Solutions, LLC

Application Performance & Productivity Team Readies Broadwell Racks for Users

- HECC's Application Performance and Productivity (APP) team ran tests and conducted performance measurements on the Broadwell racks in preparation for their release to users.
- After the Supercomputing Systems team brought up the new resources (see slide 3), the APP team began testing and found no major issues.
- The team then ran the six applications that make up the Standard Billing Unit (SBU) suite and determined a charging rate of 4.04 SBUs* for Broadwell nodes.
- The team also developed user documentation for the HECC Knowledge Base that describes the new nodes and how to use them; the Publications & Media team edited and posted the articles and updated 23 additional articles to support the Broadwell expansion.
- The APP team then organized a two-phase Early Access testing program, where users tried out new resources for free. The first phase had a limited set of users, and testing uncovered an issue with the GNU Parallel utility that was then fixed. The second phase opened up the Broadwells to all users for a full week. After the successful test period, the new nodes were released to production seeing immediate full utilization.

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node*

Mission Impact: Extensive testing involving users reduces risks associated with new system installations and improves documentation by taking into account more varied user experiences.

The Pleiades supercomputer was augmented with 14 Intel E5-2680v4 (Broadwell) racks containing 1,008 nodes, replacing 1,024 Westmere nodes. The HECC Application Performance and Productivity team's measurements show that each Broadwell node is 4.04 times more powerful than a Westmere node.

POCs: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165, NASA Advanced Supercomputing (NAS) Division; Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NAS Division, CSC Government Solutions, LLC

Security Team's Patching and Vulnerability Reporting Reduces Outstanding Patches

- The Security Team implemented weekly patch and vulnerability management processes in January 2016. Weekly reports are used by the IT support teams to identify patches and vulnerabilities for all HECC and NAS systems.
- The reports reduce risks to hosts and networks by quickly identifying vulnerabilities and missing patches that could be exploited. Results since January include:
  - One support team obtained an 83% reduction in the number of systems with outstanding vulnerabilities.
  - Another team reduced the number of outstanding patches to zero.
- These reports also:
  - Ensure hosts are in compliance with agency vulnerability and patching requirements.
  - Quickly identify vulnerabilities and missing patches that have not been addressed within the agency time requirements.
  - Help management, system owners, and systems administrators identify systems that may have not been properly patched.
  - Foster cooperative working relationship between Security and support groups: support teams provide feedback to Security about potential false-positives and status updates, and Security works with the teams to help fix vulnerabilities on their systems.

Mission Impact: By implementing weekly patch and vulnerability reporting, HECC system administrators are able to quickly identify and correct vulnerabilities and missing patches on their systems, which reduces the security risk to HECC.

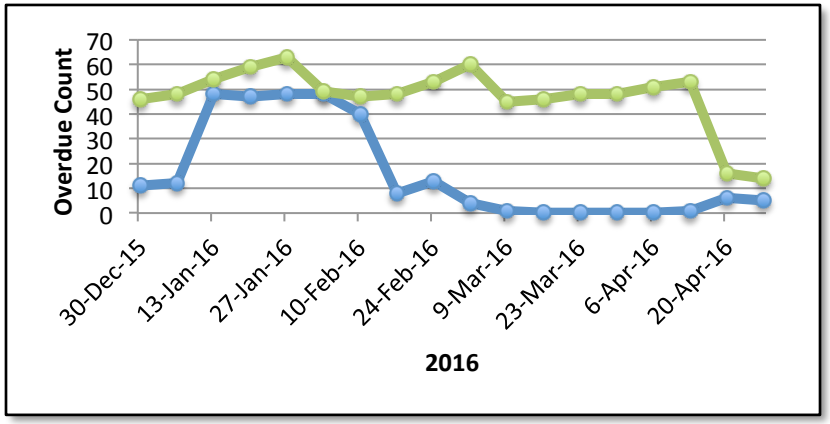


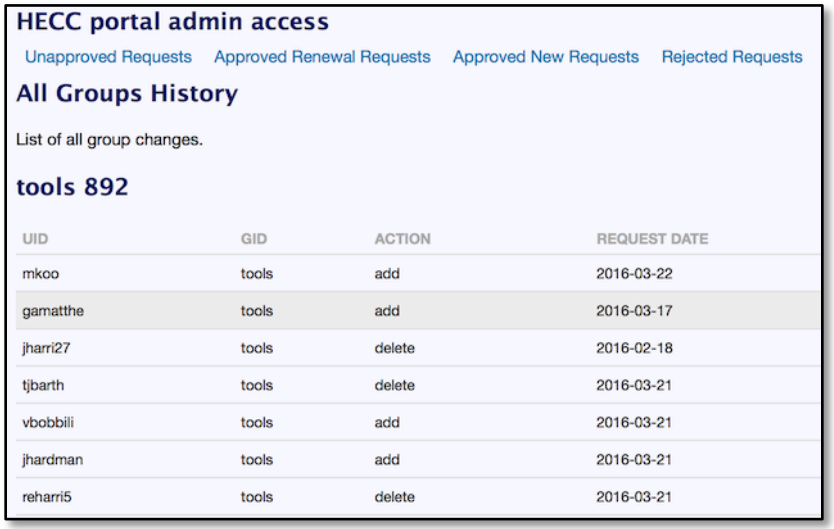
Chart showing the reduction in overdue vulnerabilities and missing patches. The chart starts in December showing a small upward trend in outstanding patches, and then shows patches decreasing once the new HECC process was put into affect. The green line represents patches for the Engineering Servers and Services team; blue represents those for the the Computing Systems team.

POCs: Tom Hinke, thomas.h.hinke@nasa.gov, (650) 604-3662, NASA Advanced Supercomputing (NAS) Division;
Derek Shaw, derek.g.shaw@nasa.gov, (650) 604-4229, NAS Division, CSC Government Solutions LLC

Capability for PIs to Add and Delete Users Added to HECC Account Request System

- The Tools team enhanced the HECC Account Request System website to allow principal investigators (PIs) to add and delete users in their groups. The PIs can now view all transactions in their group's history log.
- To manage the PI user changes, the Tools team developed a back-end system that syncs the PI website changes with the Local Account Management System (LAMS).
- They also developed a search tool to provide auto-completion of an entry based on the user's Agency User ID, first name, or last name. This ensures accurate identity of valid users without the need to provide a dropdown menu of hundreds of user names.
- The enhancement provides PIs with the capability to view and manage their groups and see real names instead of using a command-line query and getting usernames that they may not quickly associate with a particular user.

Mission Impact: HECC accounting groups are more accurately managed because the principal investigators now have the tool to manage accounts for the users in their groups.



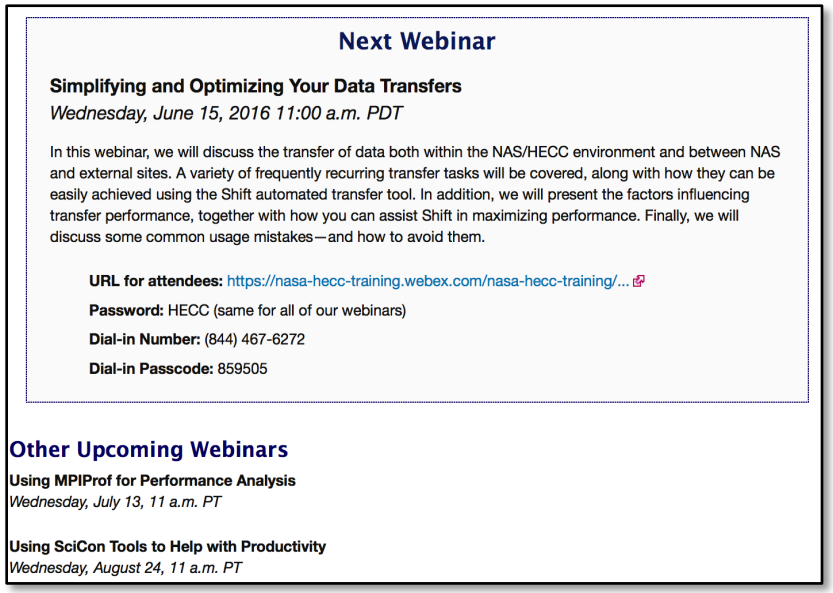
The HECC Account Request System website now provides principal investigators with their requested capabilities to manage user accounts.

POC: Ryan Spaulding, ryan.c.spaulding@nasa.gov, (408) 772-6567, NASA Advanced Supercomputing Division, ADNET Systems, Inc.

HECC Initiates New Set of User Training Webinars

- HECC User Services staff resumed the popular monthly user training webinars.
- The first webinar kicked off on Wednesday April 27 with 25 attendees. Bill Thigpen presented the topic, “HECC System Status,” covering an overview of services that are available to all users, along with future plans.
- In early May, NAS Division scientist Subhash Saini will present the topic, “Performance Evaluation of Pleiades Broadwell Nodes Using NASA Applications,” covering the architectural evolution of of five generations of Pleiades processors, trending features, and the impact of the new Broadwell processors on NASA applications.
- User Services will hold user training sessions once a month through the end of 2016. In the past, webinars were held about every two months.
- The schedule of upcoming seminars for the next thee months is posted on the HECC website: http://www.nas.nasa.gov/hecc/support/training.html
- HECC staff are planning webinars for the remainder of the year, and are also exploring other types of effective training methods.

Mission Impact: User training is one of the many capabilities offered to scientists and engineers to assist them in efficiently utilizing HECC resources for their NASA projects.



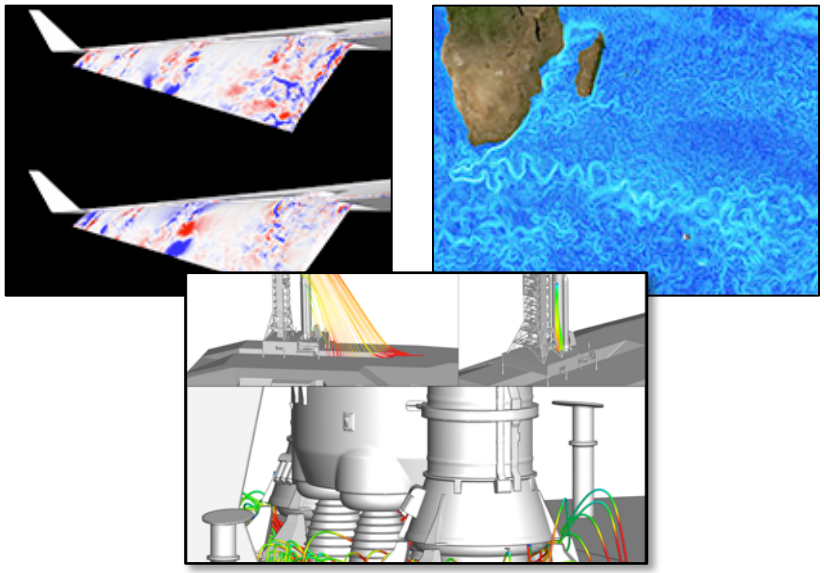
The current three-month schedule of HECC user training webinars. Users can review past slide presentations from the webinar archive on the HECC website.

POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, CSC Government Solutions LLC

April 2016 Usage on Pleiades Sets New 30-Day Record of 16.58 Million SBUs

- April usage on the Pleiades supercomputer set a new normalized (30-day-month) record.
- 16.58 million Standard Billing Units (SBUs*) were used by NASA's science and engineering organizations, exceeding the previous normalized record of 16.45 million SBUs that was set in May 2015.
- This increase was enabled by the installation of 720 of 1008 new Broadwell nodes that, upon completion in early May, will increase Pleiades' resources by 17%.
- About 330 projects from all across NASA used time on Pleiades during April.
- The top 10 projects used from 338,971 to 1,817,418 SBUs each and together accounted for over 43% of total usage.
- The HECC Project continues to plan and evaluate ways to address the current and future requirements of NASA's users.

•Mission Impact: Increasing Pleiades' system capacity provides Mission Directorates with more resources for the accomplishment of their goals and objectives.



Images from projects that were among the top users in their respective Mission Directorates. From top left:
(1) Simulated fluctuating surface pressure field on a full-scale Gulfstream aircraft during landing. *P. Moran, NASA/Ames; Airframe Noise Team, Exa Corp.*
(2) Snapshot of surface current speed in the Antarctic Circumpolar Current region. *C. Hill, MIT.*
(3) Potential debris trajectories from various parts of the launch pad and Space Launch System structures. *B. Williams, NASA Marshall.*

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node*

ESS Team Upgrades Linux Systems to 'NAStruck' Version 2 Backup Application

- HECC engineers upgraded the locally developed "NAStruck" backup application to version 2, which supports the XFS file system used in Red Hat Enterprise Linux version 7. The ESS team upgraded 250 servers and workstations to NAStruck version 2 in March 2016.
- Features of NAStruck version 2 include:
  - Support for the XFS file system.
  - Enhanced configuration file syntax allowing for default settings for client groups.
  - Ability to skip incremental dumps on systems with large data stores.
  - New command line options, bug fixes, and the backup level in the filenames.
- Future plans for this client-server application, which performs automatic, unattended daily backups, include providing support for the supercomputers at the NASA Advanced Supercomputing (NAS) facility.

Mission Impact: The latest version of the NAStruck application provides HECC systems engineers with the capability to back up systems that are being upgraded to the latest Red Hat version.

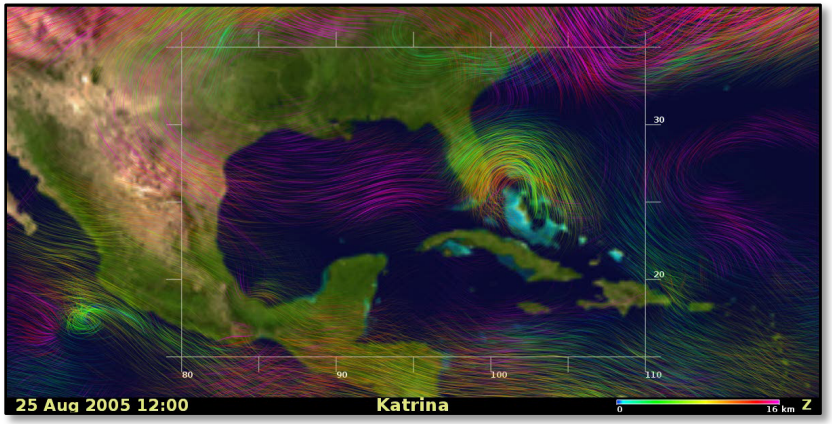
Through the locally developed NAStruck application, HECC Linux servers and workstations are backed up to the archive tape storage systems (pictured above) at the NASA Advanced Supercomputing (NAS) facility.

POCs: Frank Cianci, frank.cianci@nasa.gov, (650) 604-2559, NASA Advanced Supercomputing (NAS) Division, ADNET Systems, Inc.; Iain Morgan, iain.morgan@nasa.gov, (650) 604-4492, NAS Division, Stinger Ghaffarian Technologies, Inc.

Using Katrina and Sandy Data to Improve Hurricane Prediction Tools *

- Using data from Hurricanes Katrina (2005) and Sandy (2012), researchers at San Diego State University (SDSU) ran large-scale simulations on Pleiades to study the role of multiscale processes associated with environmental flows and improve prediction capabilities for high-impact tropical cyclones (TCs).
- The SDSU team deployed NASA's Coupled Advanced global Modeling & Visualization (CAMVIS) framework and Multiscale Analysis Package (MAP) to obtain the following:
  - Accurate 5-day track and intensity predictions and high-fidelity 3D visualizations for Katrina, showing multiscale interactions with an approaching upper-level trough that may have led to the storm's intensification prior to landfall.
  - Realistic 7-day track and 6-day genesis simulations of Sandy; multiscale analysis and high-fidelity visualizations revealed the multiscale processes of Sandy's formation and movement.
  - Multiscale analysis with MAP's parallel ensemble empirical mode decomposition capability revealed the role of tropical waves, westerly wind belt, and a Madden-Julian Oscillation in Sandy's initial formation.
- The SDSU team is now running multi-TC genesis simulations and analyzing results to understand how downscaling and upscaling processes may help predict TCs in numerical models.

Mission Impact: HECC supercomputing technologies and integrated services make it feasible for scientists to improve large-scale analysis tools for better understanding and prediction of hurricanes, which in turn may save lives and reduce damage costs.



This four-dimensional (X-Y-Z-time) visualization from a multiscale simulation for Hurricane Katrina (2005) shows the horizontal phasing of an approaching jet stream (upper left corner) and Katrina's southwesterly outflow (to the southeast of the jet) prior to landfall. The phasing further strengthens the upper-level anticyclonic flow over the hurricane (dense, streamlines in expanding pink at right), enhancing Katrina's development and creating strong, deep convections. *Bron Nelson, NASA/Ames*

POC: Bo-Wen Shen, bshen@mail.sdsu.edu, (619) 594-5962, San Diego State University

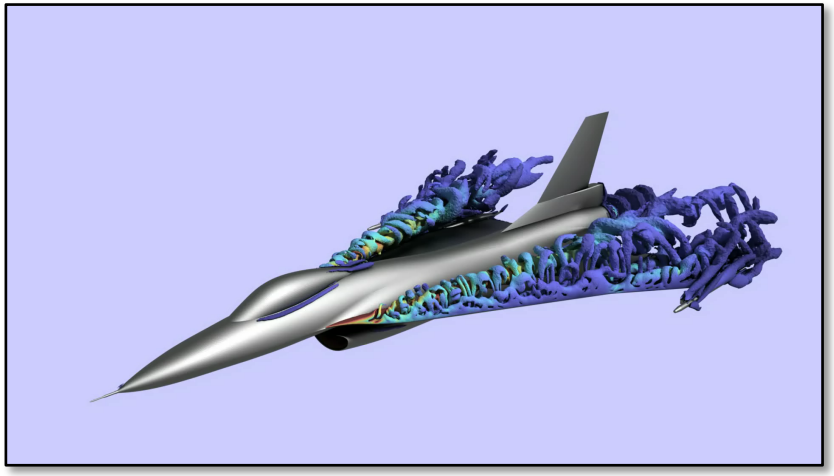
** HECC provided supercomputing resources and services in support of this work*

Developing FUN3D for High-Fidelity Physics-Based Analysis & Design of Complex Configurations *

- Researchers at NASA Langley are running simulations on Pleiades to advance the development of FUN3D, an unstructured-grid computational fluid dynamics suite of codes that provides a wide range of modeling tools for design and analysis of next-generation flight vehicles.
- Due to its unique capabilities and performance on large-scale computing platforms, FUN3D is used widely by numerous NASA programs, the aerospace industry, the U.S. Department of Defense, and over 100 universities for research. Several recent applications of FUN3D include:
  - NASA programs including fixed-wing and rotary wing vehicle design, sonic boom mitigation, and the development of the new Space Launch System.
  - Development of commercial crew spacecraft at companies such as SpaceX.
  - Development of efficient green energy concepts, such as distributed electric propulsion and wind turbines.
- FUN3D has been a key factor in developing adjoint-based methods for mesh adaptation and error estimation, reducing the uncertainties in accuracy typically present in numerical simulations.

** HECC provided supercomputing resources and services in support of this work*

Mission Impact: FUN3D is widely used by numerous NASA programs including fixed- and rotary-wing vehicle design, sonic boom mitigation, and SLS development. HECC resources enable the simultaneous solution of billions of equations, which is required by FUN3D simulations.

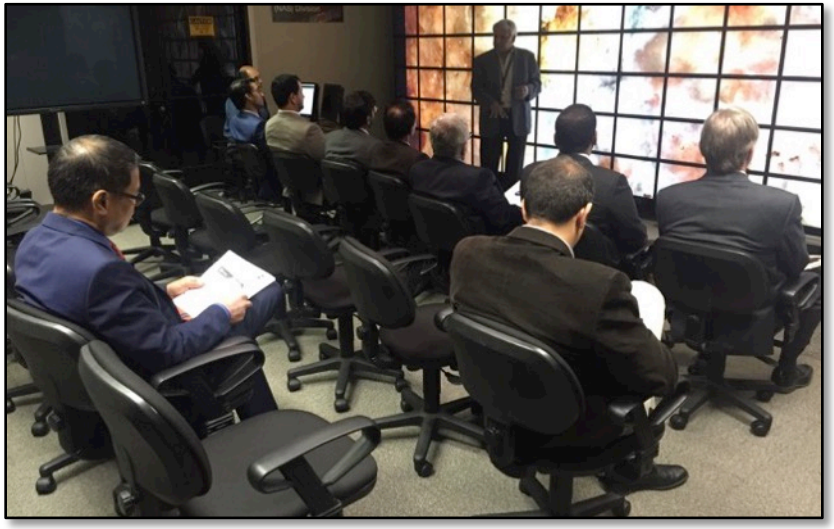


Visualization of a computational fluid dynamics simulation of an F-16XL aircraft at a low-speed, high angle-of-attack position. The hybrid Reynolds-averaged Navier-Stokes large eddy simulation was run using FUN3D. *Tim Sandstrom, NASA/Ames*

POCs: Kyle Anderson, william.k.anderson@nasa.gov, (757) 864-9195, Eric Nielsen, eric.j.nielsen@nasa.gov, (757) 864-2239, NASA Langley Research Center

HECC Facility Hosts Several Visitors and Tours in April 2016

- HECC hosted 9 tour groups in April; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  - Heraldo Muñoz, director, Energy, Science and Technology, Chilean Ministry of Foreign Affairs.
  - Mohammed Al Ahbabi, director general, United Arab Emirates Space Agency.
  - David Bowles, director, NASA Langley Research Center, who was briefed by NAS Division managers on our supercomputing facility and taken on a facility tour.
  - A group of managers of the Royal Institute of Technology (KTH) in Stockholm.
  - Students from the Blue Marble Space Institute of Science, Young Scientist Program.
  - A group of researchers who participated in the NASA Ames Space Portal Technology Day.



Piyush Mehrotra, NAS division chief, gave an overview of the HECC project and a hyperwall demonstration to a combined group of guests that included Mohammed Al Ahbabi, United Arab Emirates Space Agency, and his staff, and Heraldo Munoz, Chilean Ministry of Foreign Affairs.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers

- "**Turbulent Chemical Diffusion in Convectively Bounded Carbon Flames**," D. Lecoanet, et al. arXiv:1603.08921 [astro-ph.SR], March 29, 2016. * *http://arxiv.org/abs/1603.08921*
- "**A Population of Short-Period Variable Quasars from PTF as Supermassive Black Hole Binary Candidates**," M. Charisi, et al., arXiv:1604.01020 [astro-ph.GA], April 4, 2016. * *http://arxiv.org/abs/1604.01020*
- "**The Impact of Stellar Feedback on Hot Gas in Galaxy Haloes: the Sunyaev-Zel'dovich Effect and Soft X-Ray Emission**," F. van de Voort, et al., arXiv:1604.01397 [astro-ph.GA], April 5, 2016. * *http://arxiv.org/abs/1604.01397*
- "**Effects of Variations in Electron Thermal Velocity on the Whistler Anisotropy Instability: Particle-in-Cell Simulations**," R. S. Hughes, J. Wang, V. Decyk, S. P. Gary, Physics of Plasmas, vol. 23, no.4, April 18, 2016. * *http://scitation.aip.org/content/aip/journal/pop/23/4/10.1063/1.4945748*
- "**Developing Atmospheric Retrieval Methods for Direct Imaging Spectroscopy of Gas Giants in Reflected Light I: Methane Abundances and Basic Cloud Properties**," R. Lupu, et al., arXiv:1604.05370 [astro-ph.IM], April 18, 2016.* *http://arxiv.org/abs/1604.05370*

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Modeling the Initiation of the 2006 December 13 Coronal Mass Ejection in AR 10930: the Structure and Dynamics of the Erupting Flux Rope**," Y. Fan, arXiv:1604.05687 [astro-ph.SR], April 19, 2016. *
  http://arxiv.org/abs/1604.05687
- "**Detection of Potential Transit Signals in 17 Quarters of Kepler Data: Results of the Final Kepler Mission Transiting Planet Search (DR25)**," J. Twicken, et al. arXiv: 1604.06140 [astro-ph.EP], April 20, 2016. *
  http://arxiv.org/abs/1604.06140

** HECC provided supercomputing resources and services in support of this work*

Presentations

- "**HECC—Moving to the Future, Today**," W. Thigpen, Plenary Presenter at the 7th International Supercomputing Conference in Mexico (ISUM), Puebla, Mexico, April 11-13, 2016.

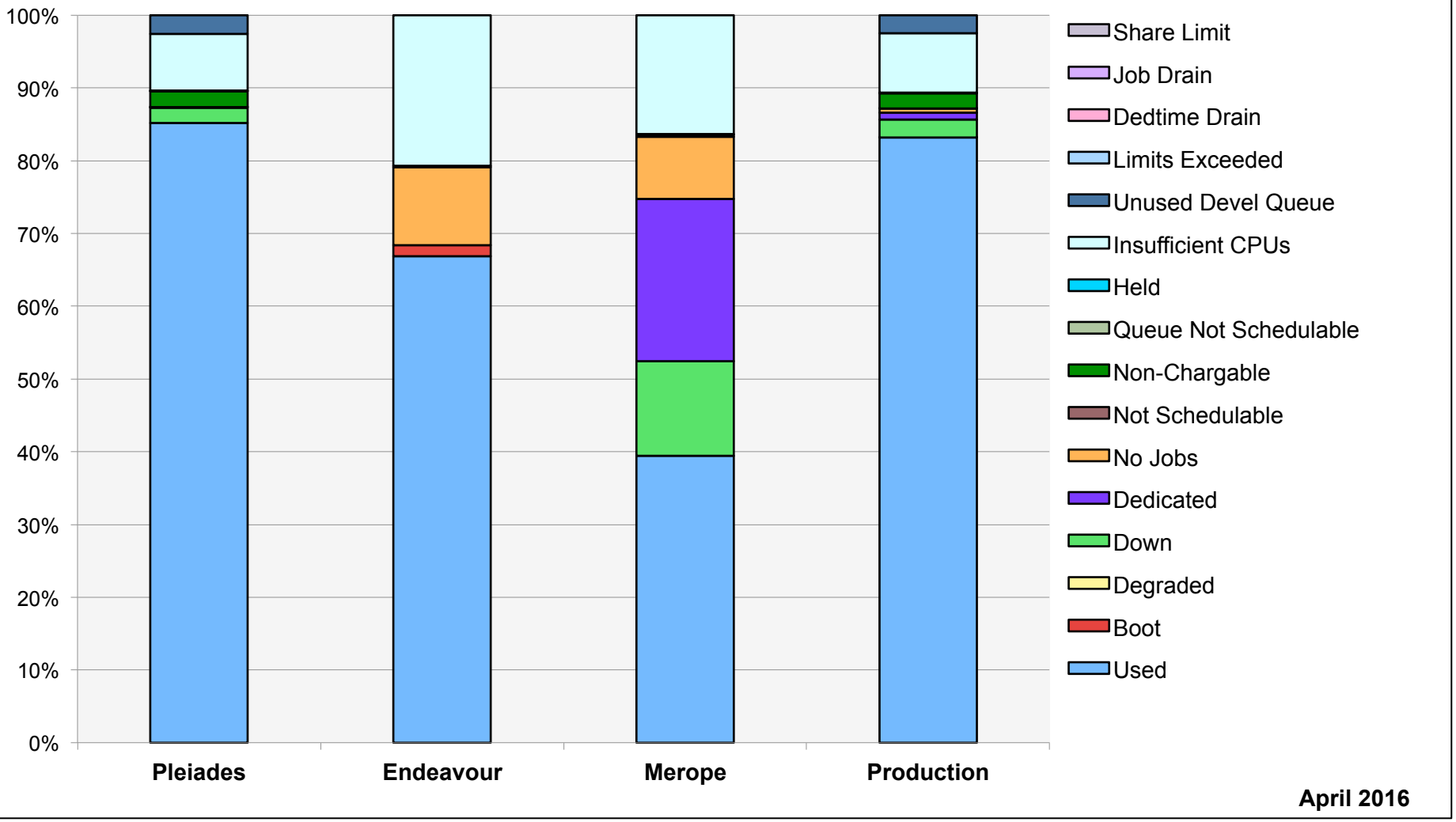
News and Events

- **Tooling Up for Cleaner Skies, Quieter Aircraft**, *NAS feature story*, April 12, 2016—NASA's Environmentally Responsible Aviation program is studying green aviation technologies to improve aircraft fuel efficiency, reduce carbon emissions, and meet noise restriction standards. Researchers in the NAS Division are simulating a contra-rotating open rotor technology using their in-house Launch Ascent and Vehicle Aerodynamics (LAVA) software framework.
  http://www.nas.nasa.gov/publications/articles/feature_openrotor_Kiris.html
  - **NASA Supercomputer Simulations Help Improve Aircraft Propulsion Design**, *NASA Ames video feature,* April 12, 2016.
    http://www.nasa.gov/image-feature/ames/nasa-supercomputer-simulations-help-improve-aircraft-propulsion-design
  - **Fiery Furnace Galaxies, Fair Fungal Partners and Zika on the Brain**, *Cosmos Magazine*, April 15, 2016 ("NASA supercomputer simulations improve aircraft design," featured as part of weekly roundup).
    https://cosmosmagazine.com/technology/fiery-furnace-galaxies-fair-fungal-partners-and-zika-brain
  - **This Week in Technology, April 25-29, 2016**, *Aviation Week,* April 25, 2016 (featured as part of weekly roundup, subscription required to view).
    http://aviationweek.com/commercial-aviation/week-technology-april-25-29-2016

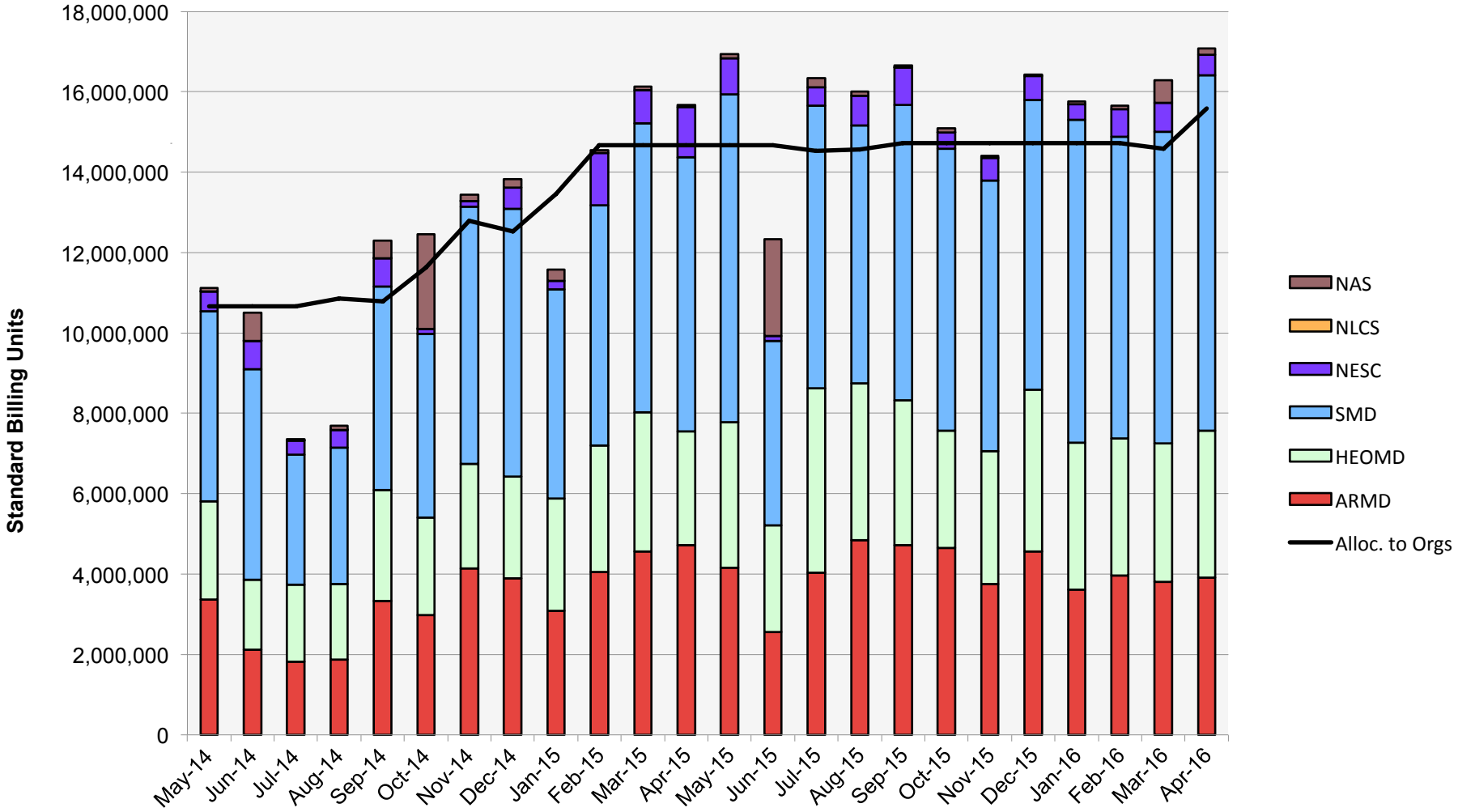
News and Events (cont.)

- **NASA's Fermi Telescope Poised to Pin Down Gravitational Wave Sources**, *NASA Goddard Feature*, April 18, 2016—Using the Pleiades supercomputer, NASA researchers simulated the merger of two black holes, modeling the September 14 gravitational wave detection by LIGO and NASA's Fermi space telescope. (Visualization of merging black holes and gravitational waves developed by HECC experts.) *http://www.nasa.gov/feature/goddard/2016/nasas-fermi-telescope-poised-to-pin-down-gravitational-wave-sources*
- **Exascale Storage Targets Big Data Archives**, *Datanami,* April 21, 2016—Spectra Logic unveils its exascale tape storage system, which has been installed at the NAS facility and increases the facility's tape storage capacity to half-an-exabyte of archival storage. *http://www.datanami.com/2016/04/21/exascale-storage-targets-big-data-archives/*

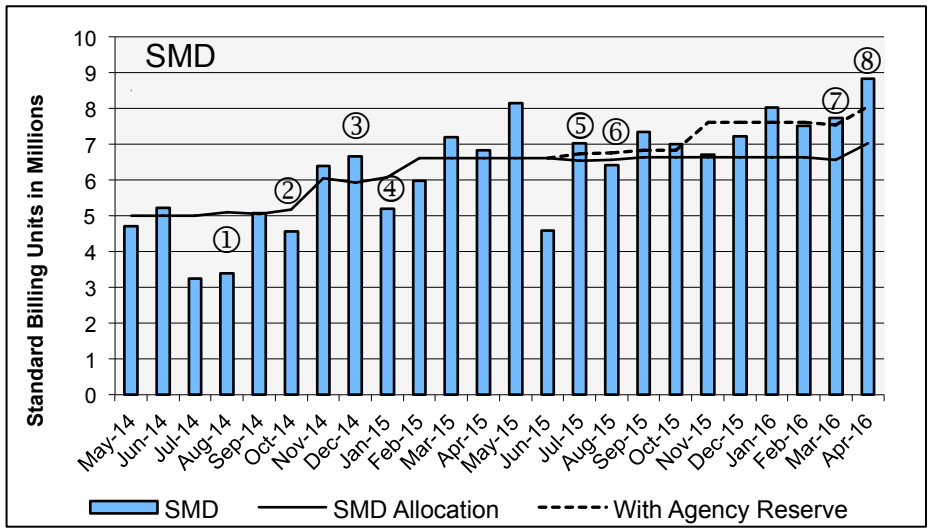
HECC Utilization

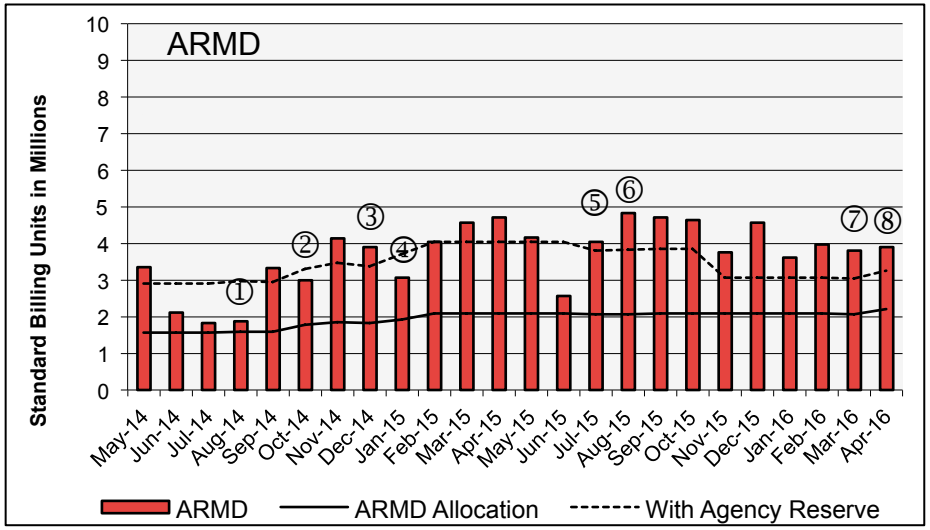


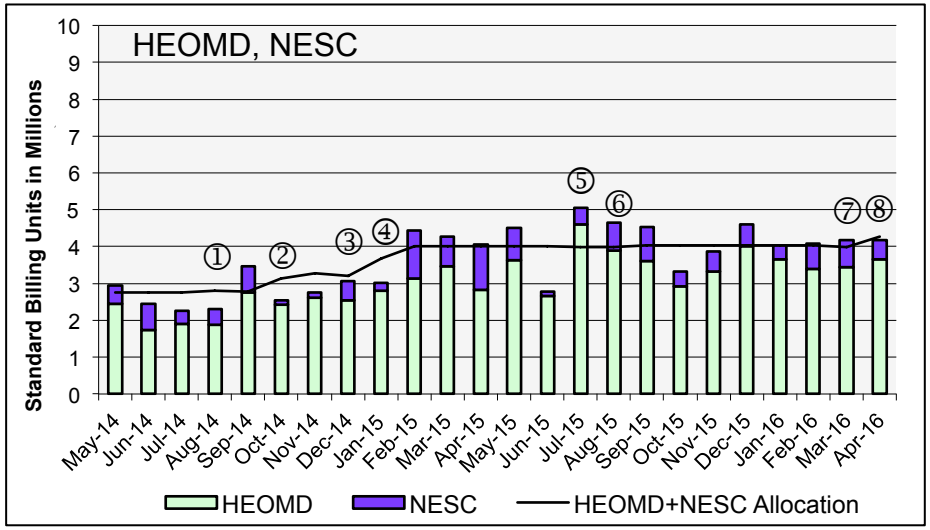
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 6 Westmere Racks added to Merope, Merope Harpertown retired

② 16 Westmere Racks retired, 3 Ivy Bridge Racks added, 15 Haswell Racks added to Pleiades; 10 Nehalem Racks and 2 Westmere Racks added to Merope

③ 16 Westmere Racks retired from Pleiades

④ 14 Haswell racks added to Pleiades

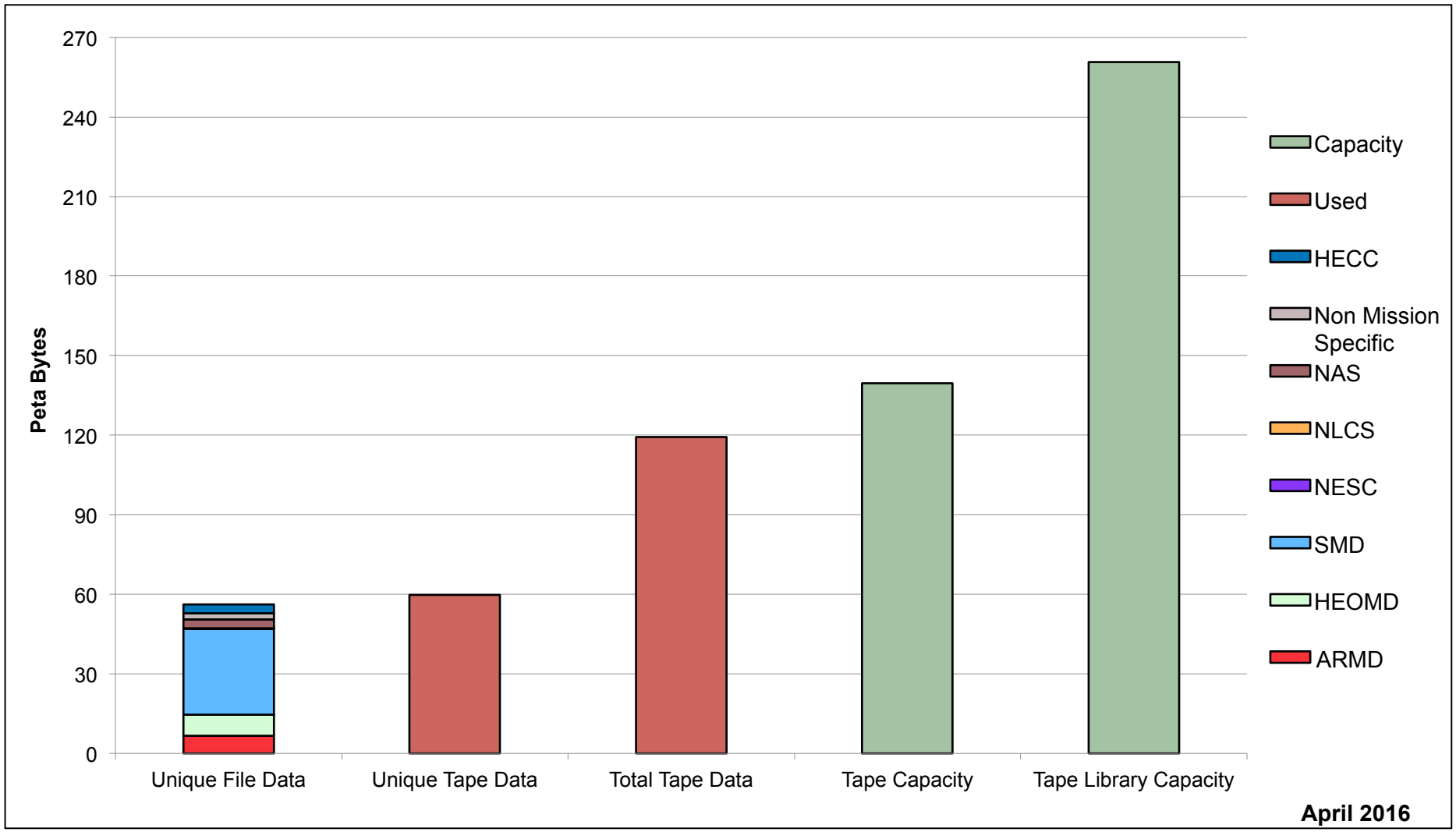
⑤ 7 Merope Nehalem Racks removed from Merope

⑥ 7 Merope Westmere Racks added to Merope

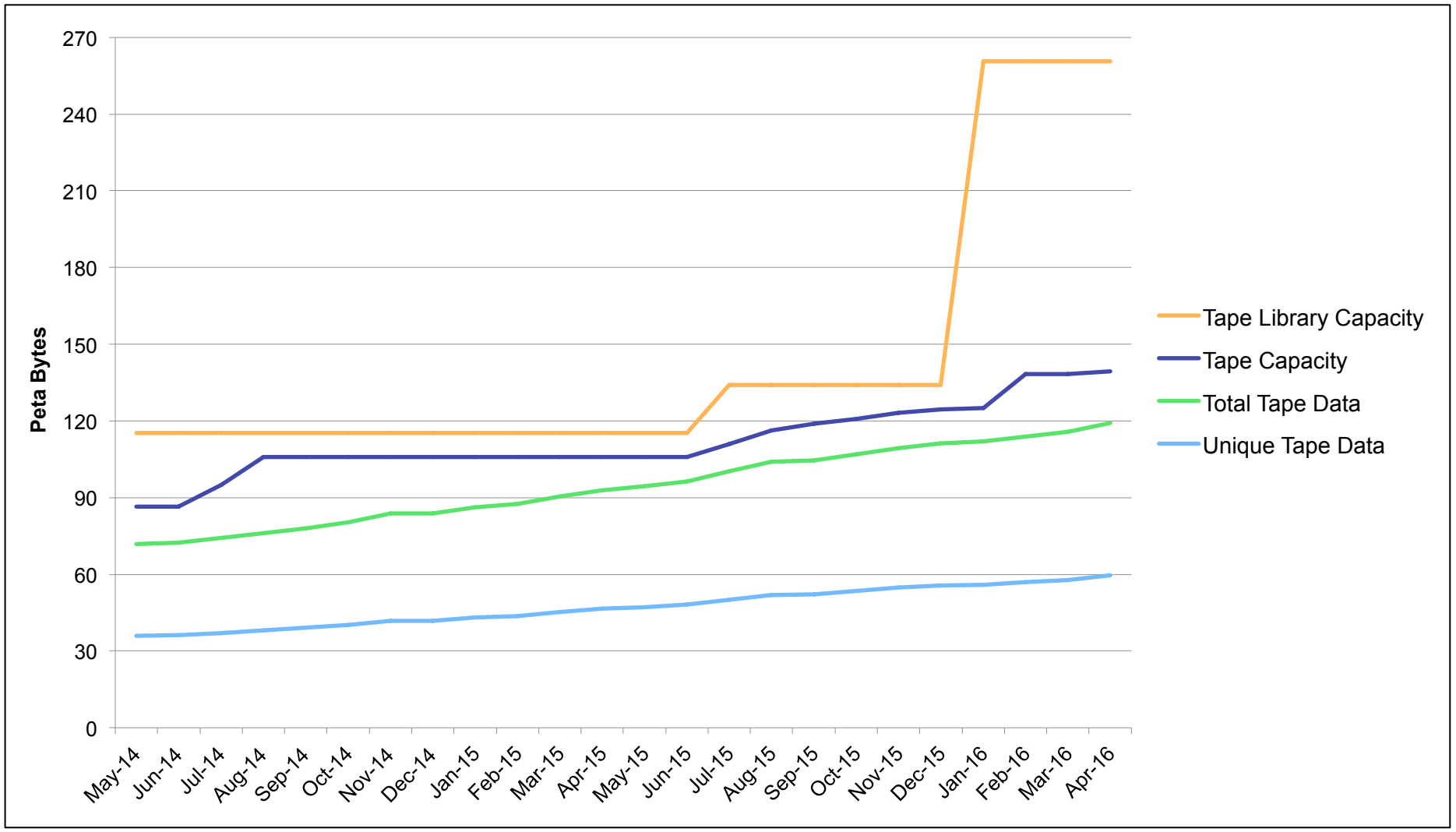
⑦ 16 Westmere Racks retired from Pleiades

⑧ 10 Broadwell Racks added to Pleiades

Tape Archive Status

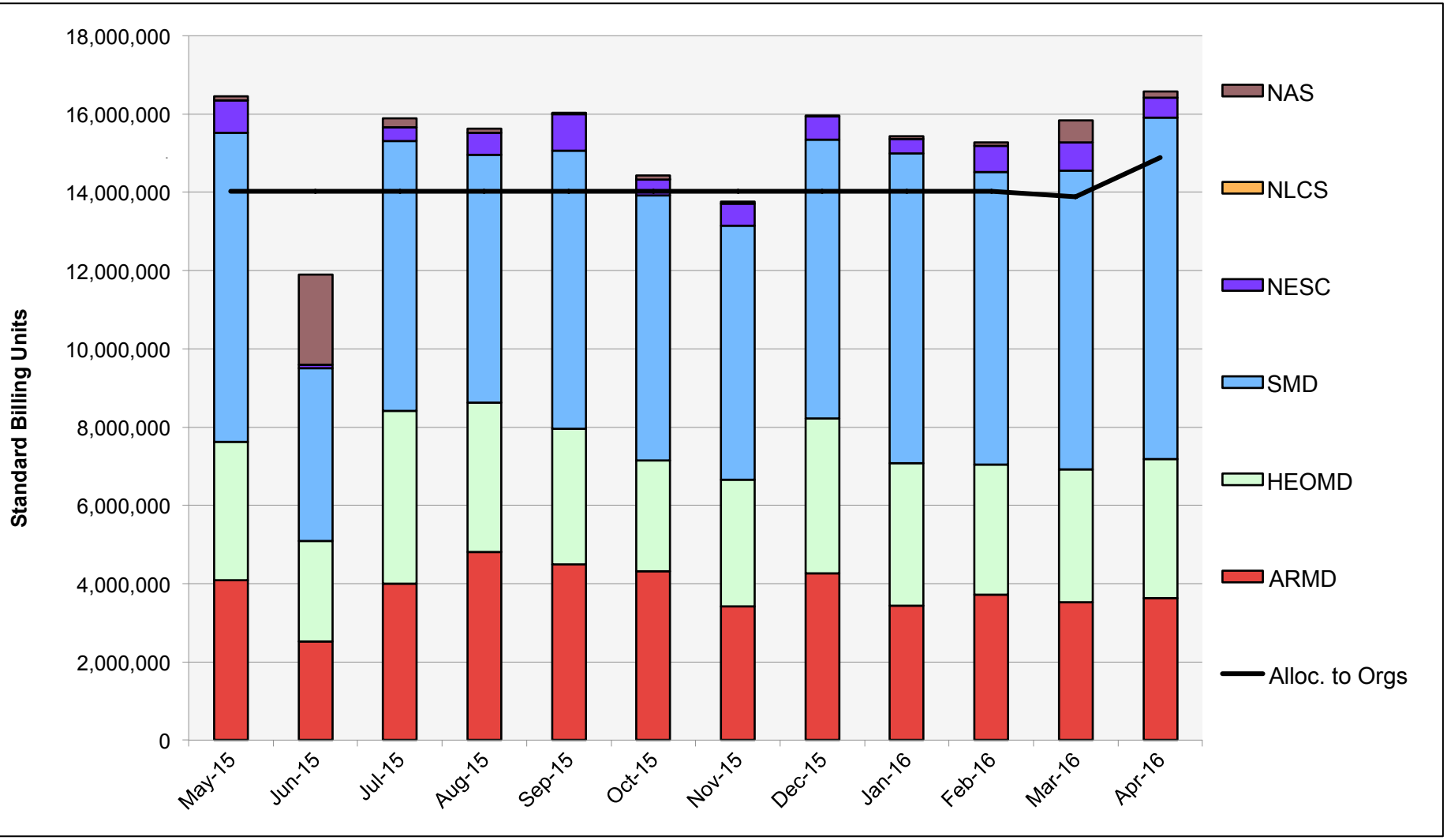


Tape Archive Status

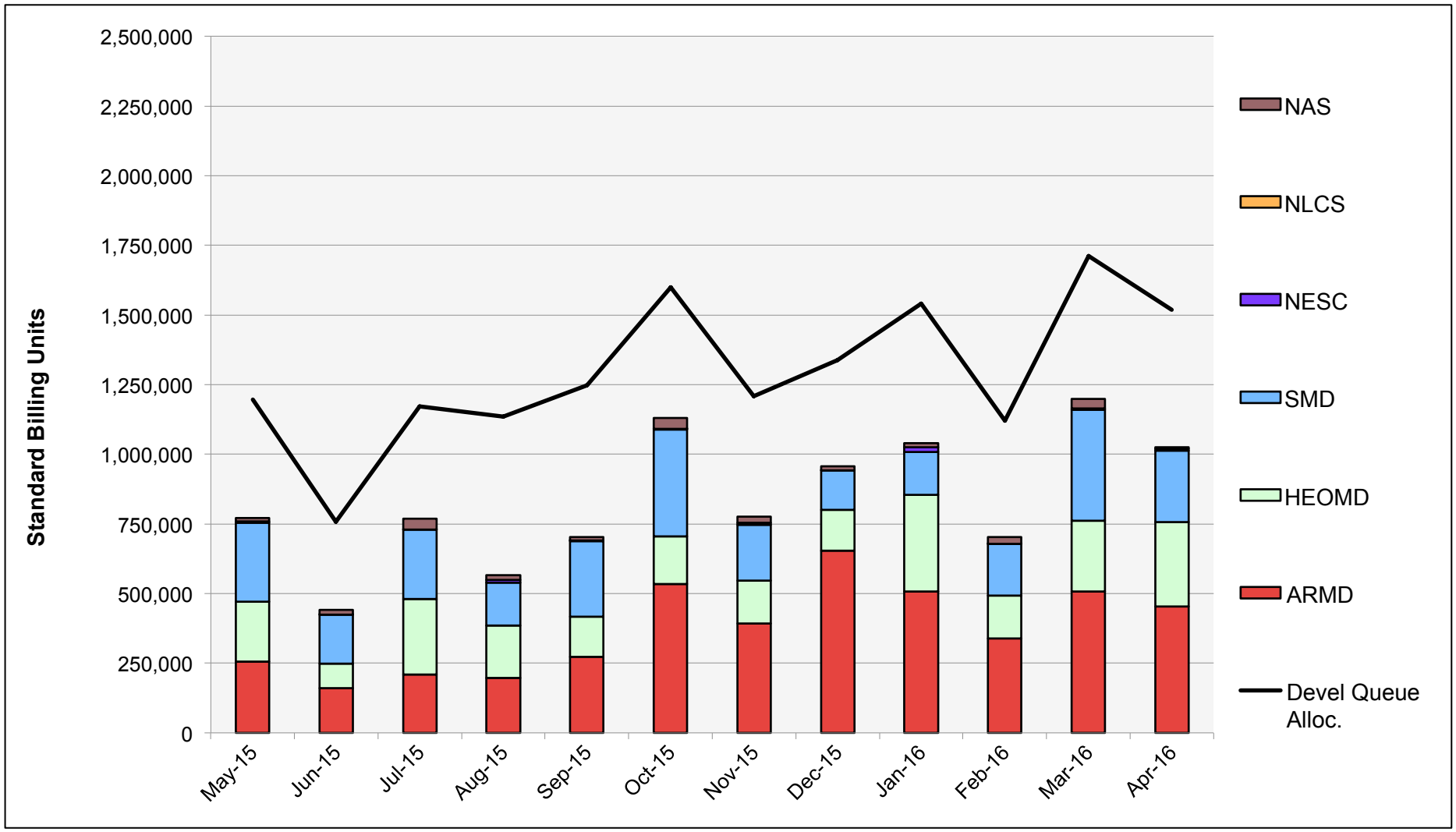


Note that when the LTO-5 drives are replaced with the existing LTO-7 drives, the capacity will rise to 490 PB

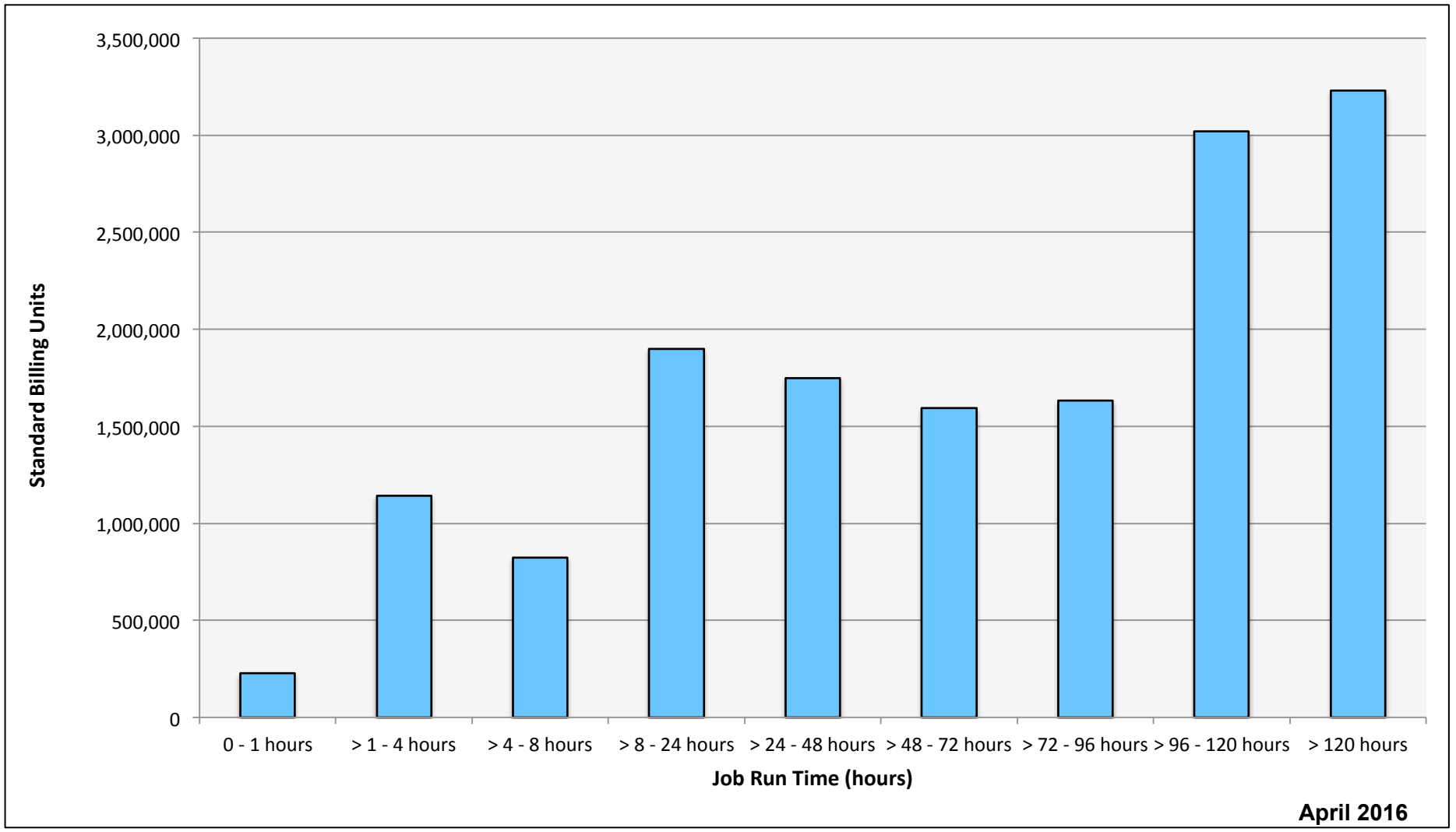
Pleiades:
SBUs Reported, Normalized to 30-Day Month



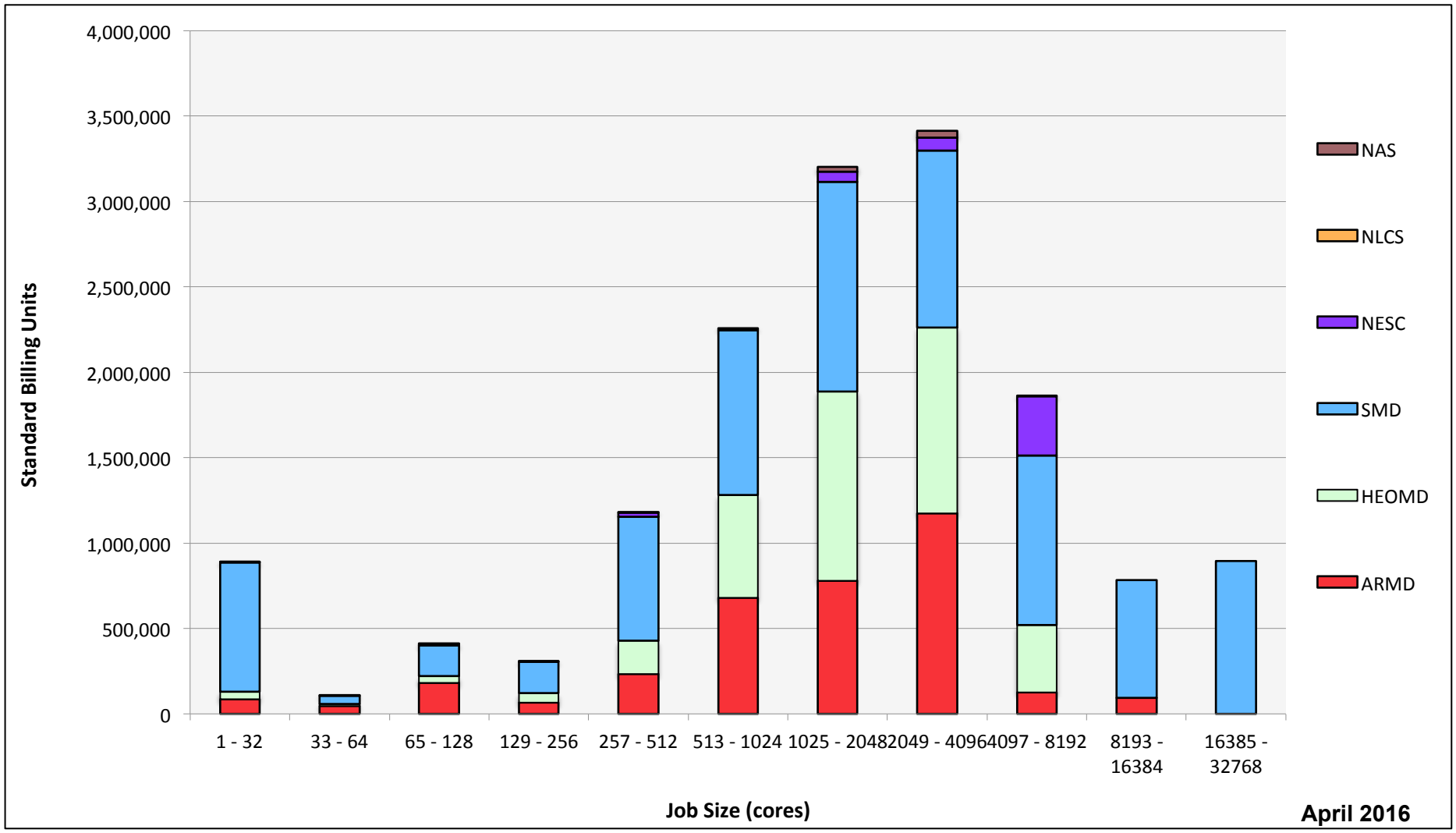
Pleiades:
Devel Queue Utilization



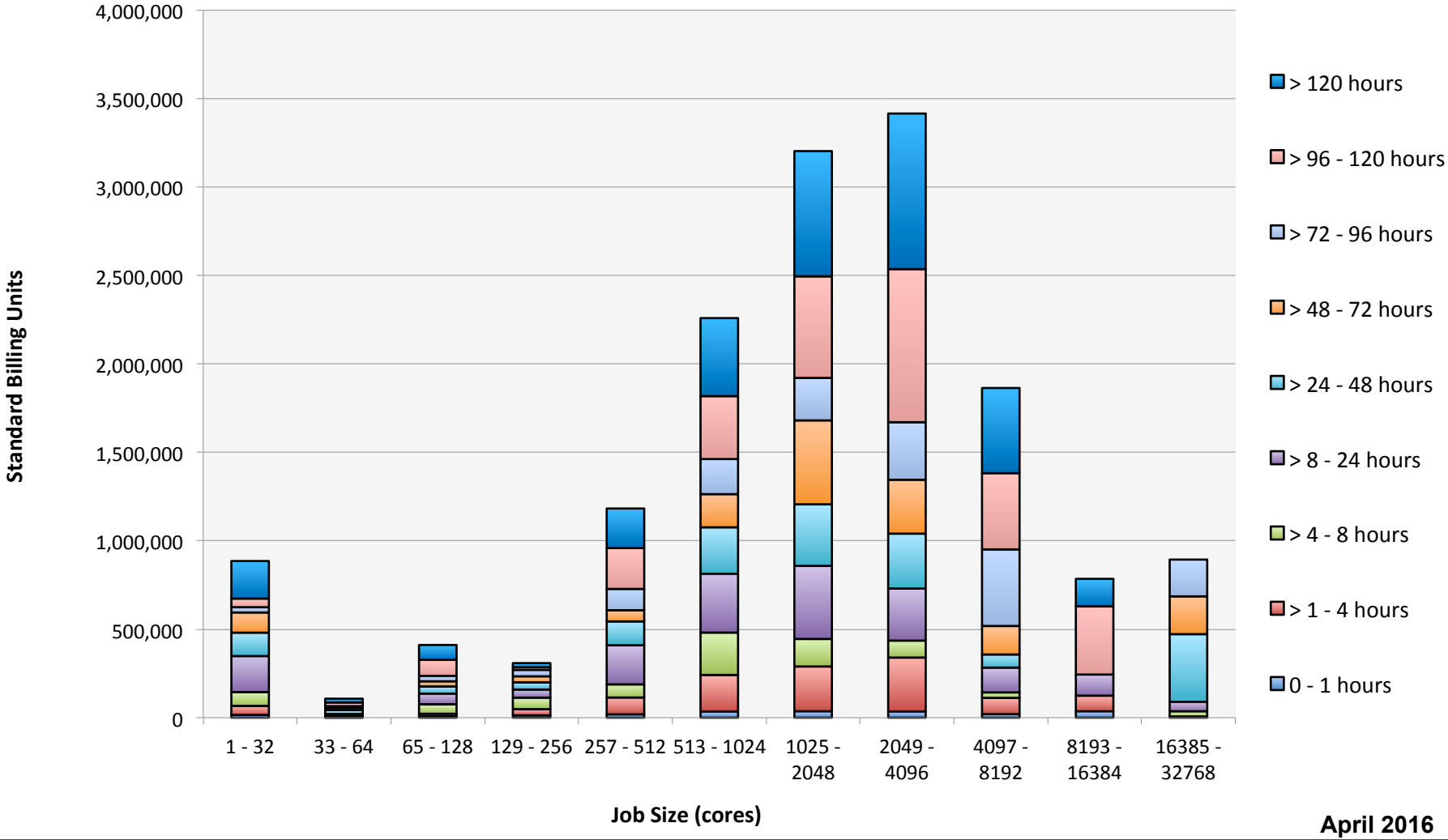
Pleiades:
Monthly Utilization by Job Length



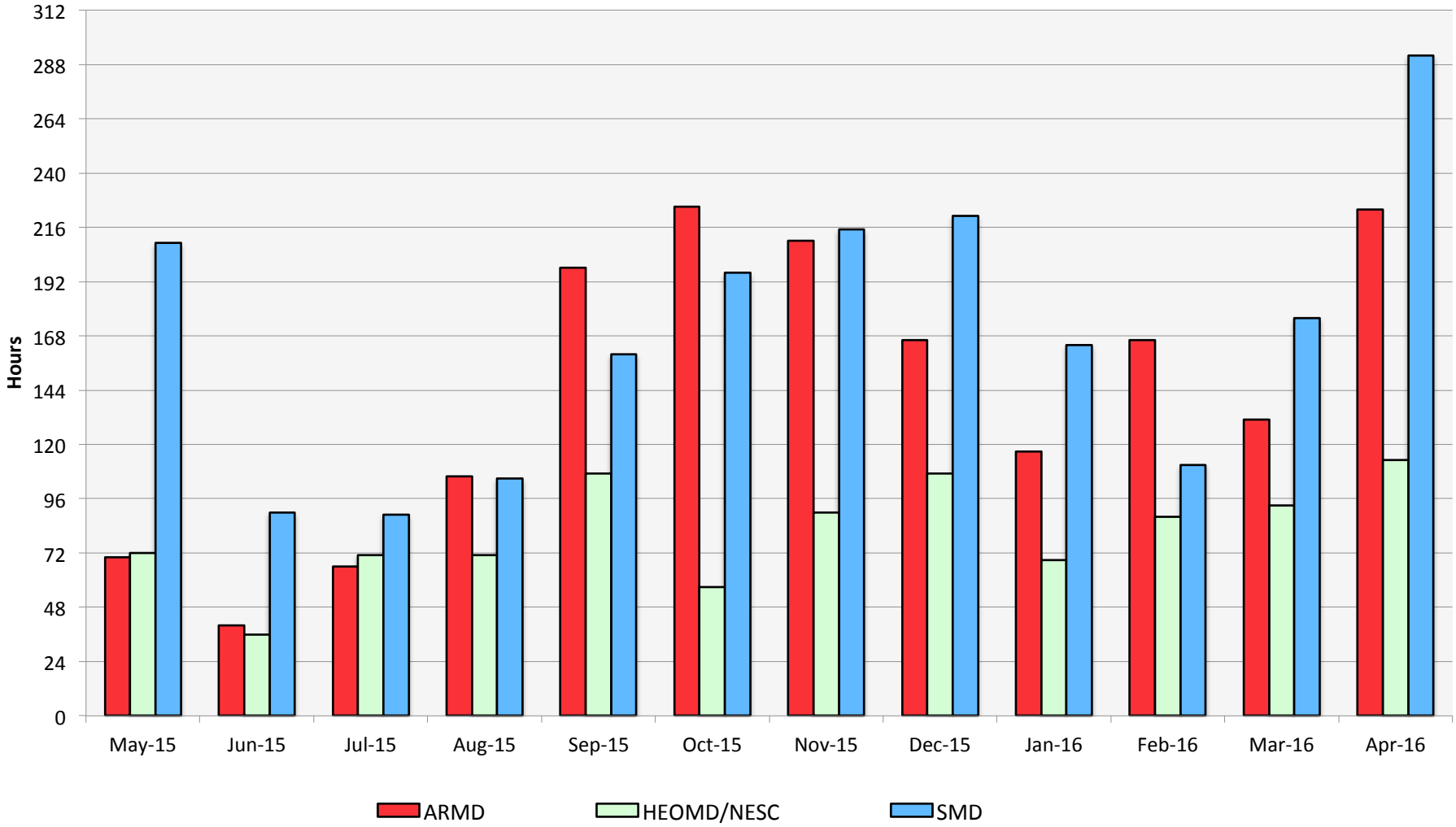
Pleiades:
Monthly Utilization by Size and Mission



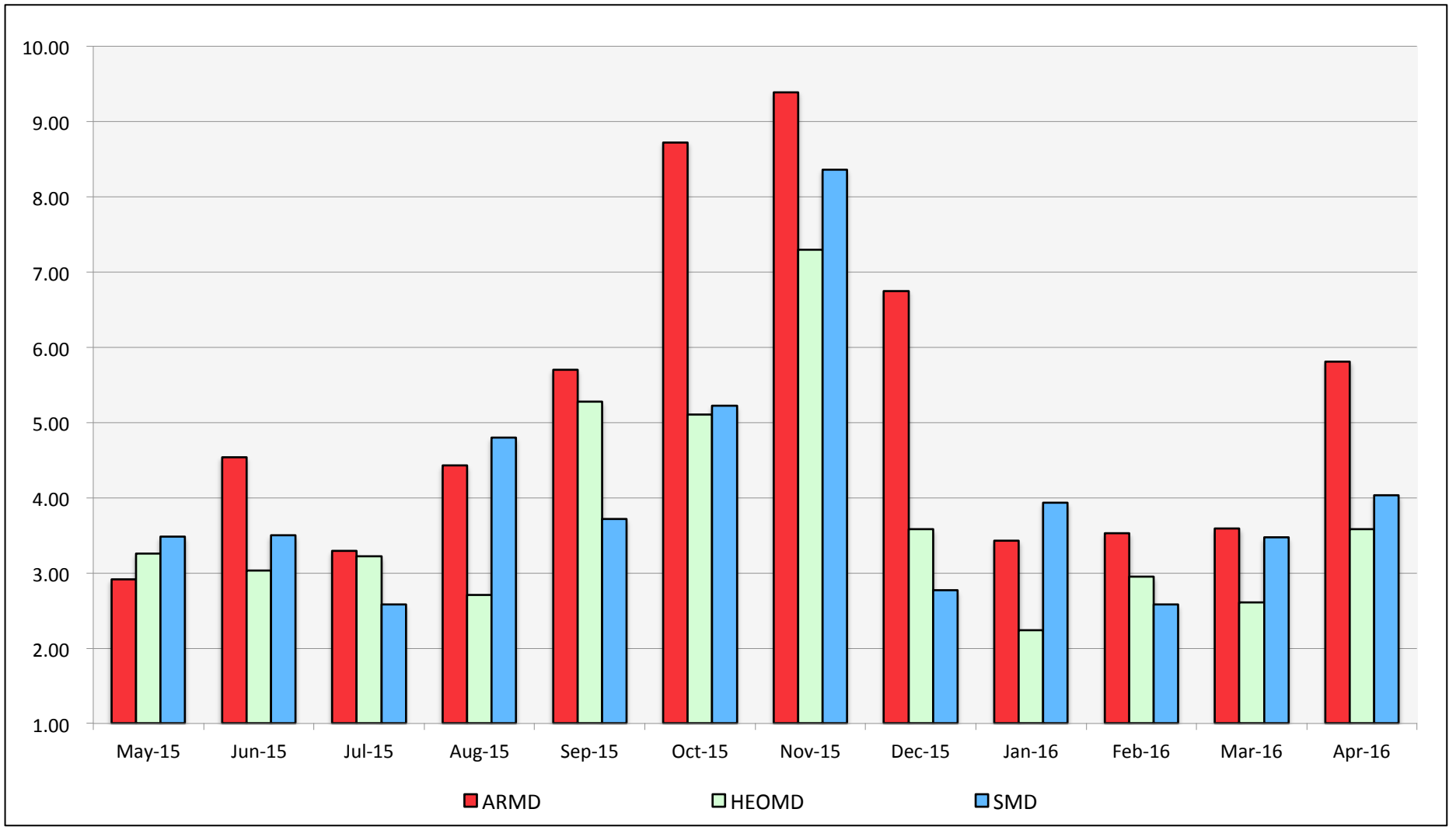
Pleiades:
Monthly Utilization by Size and Length



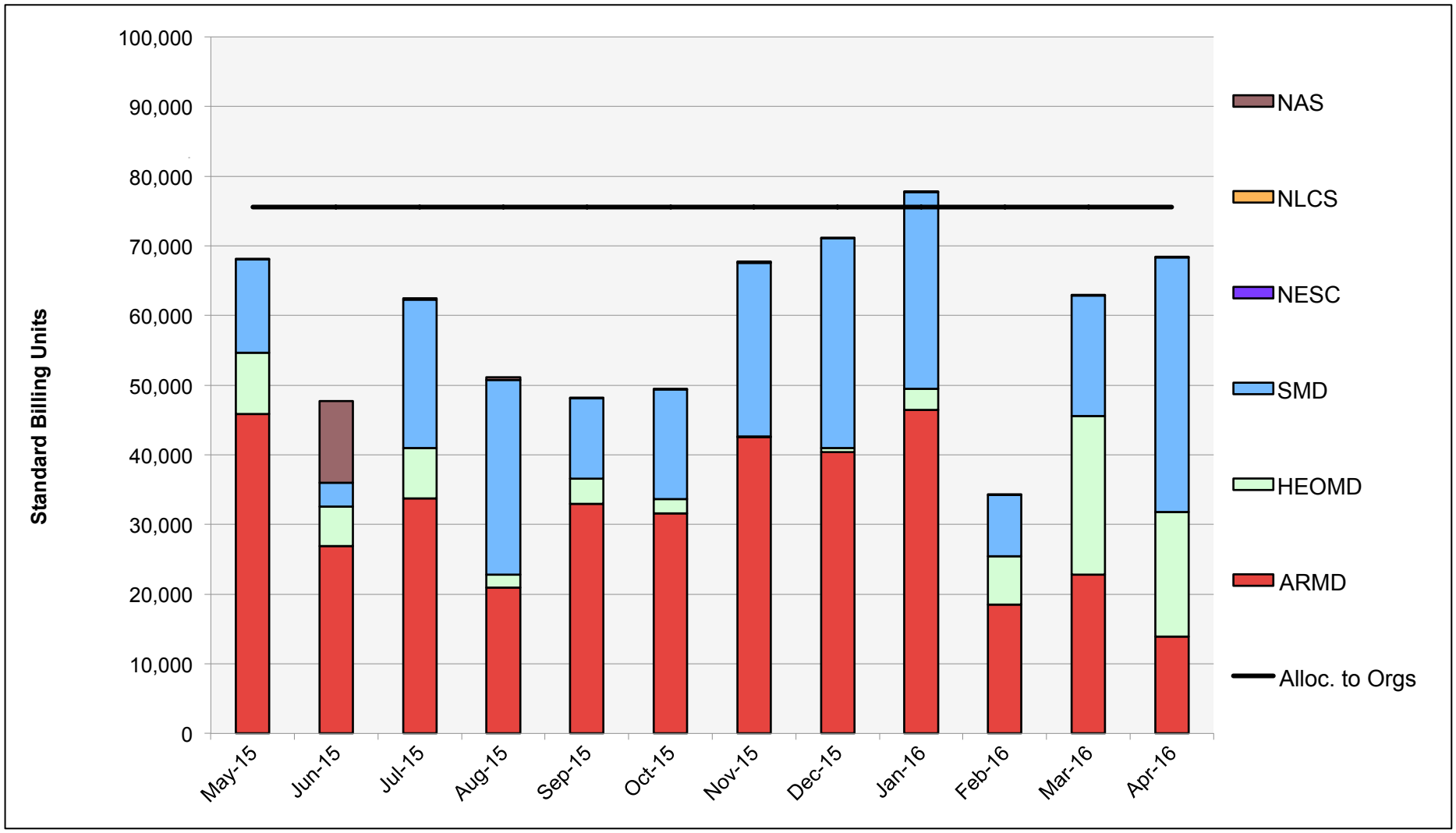
Pleiades:
Average Time to Clear All Jobs



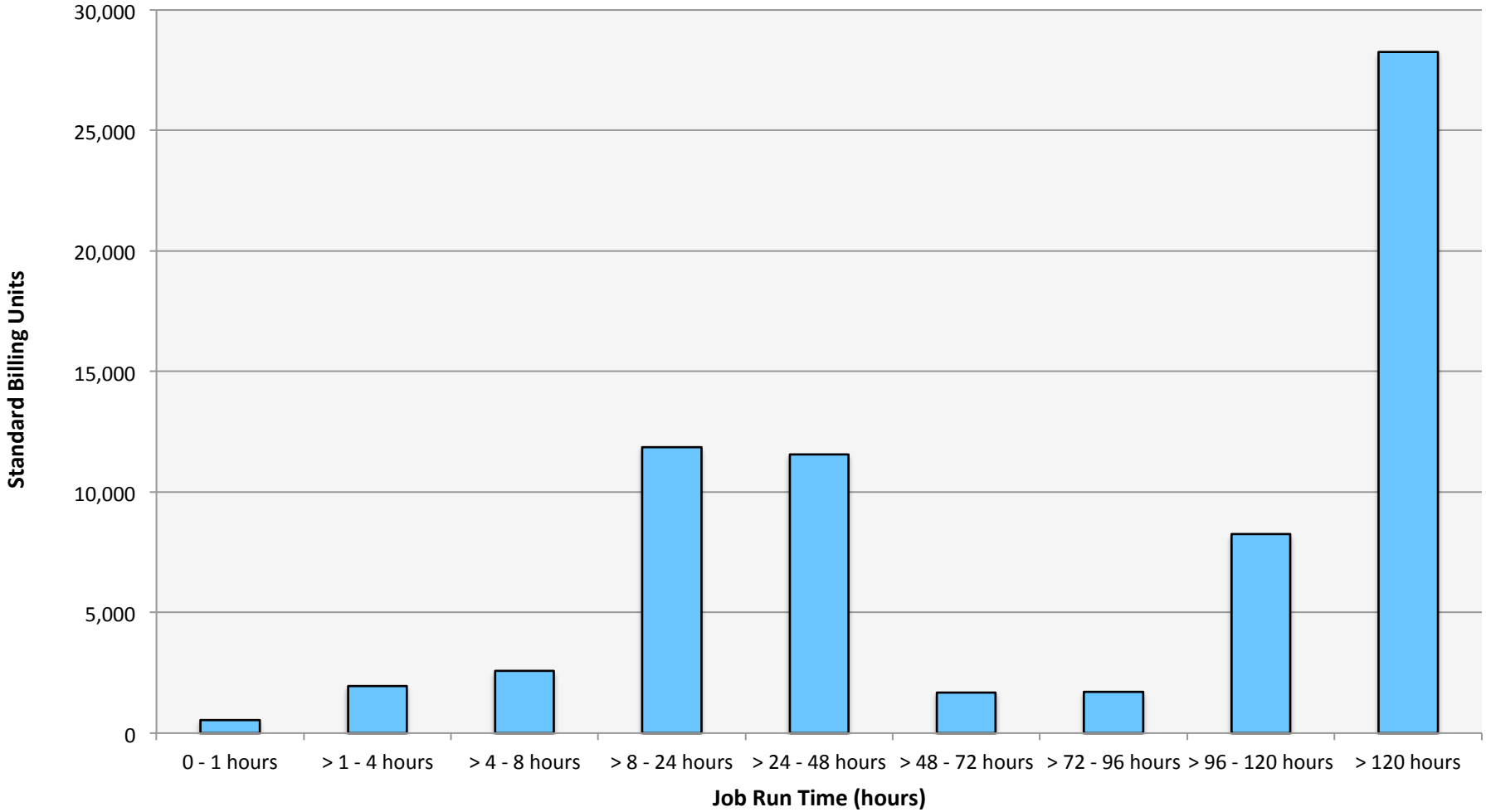
Pleiades:
Average Expansion Factor



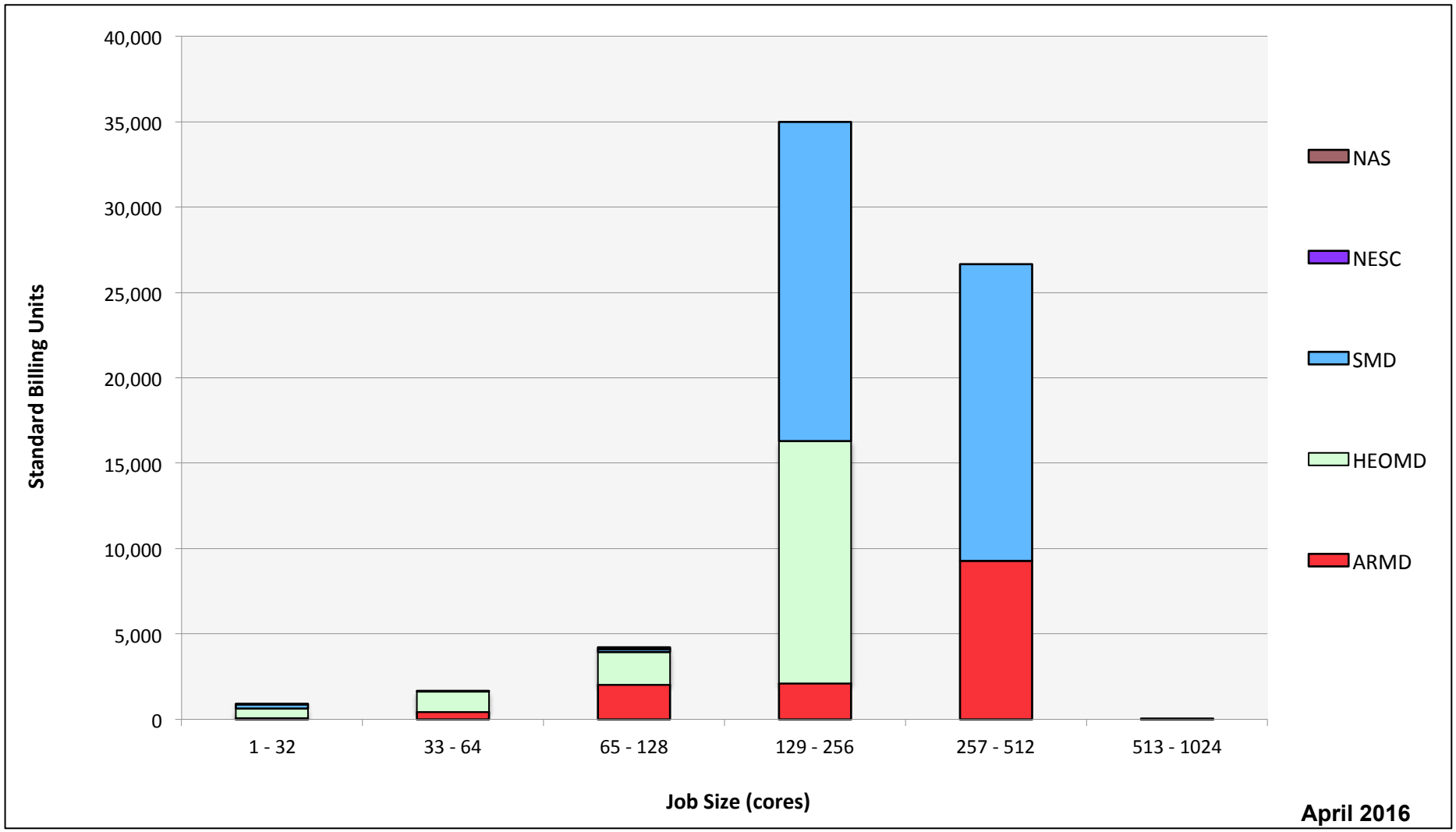
Endeavour:
SBUs Reported, Normalized to 30-Day Month



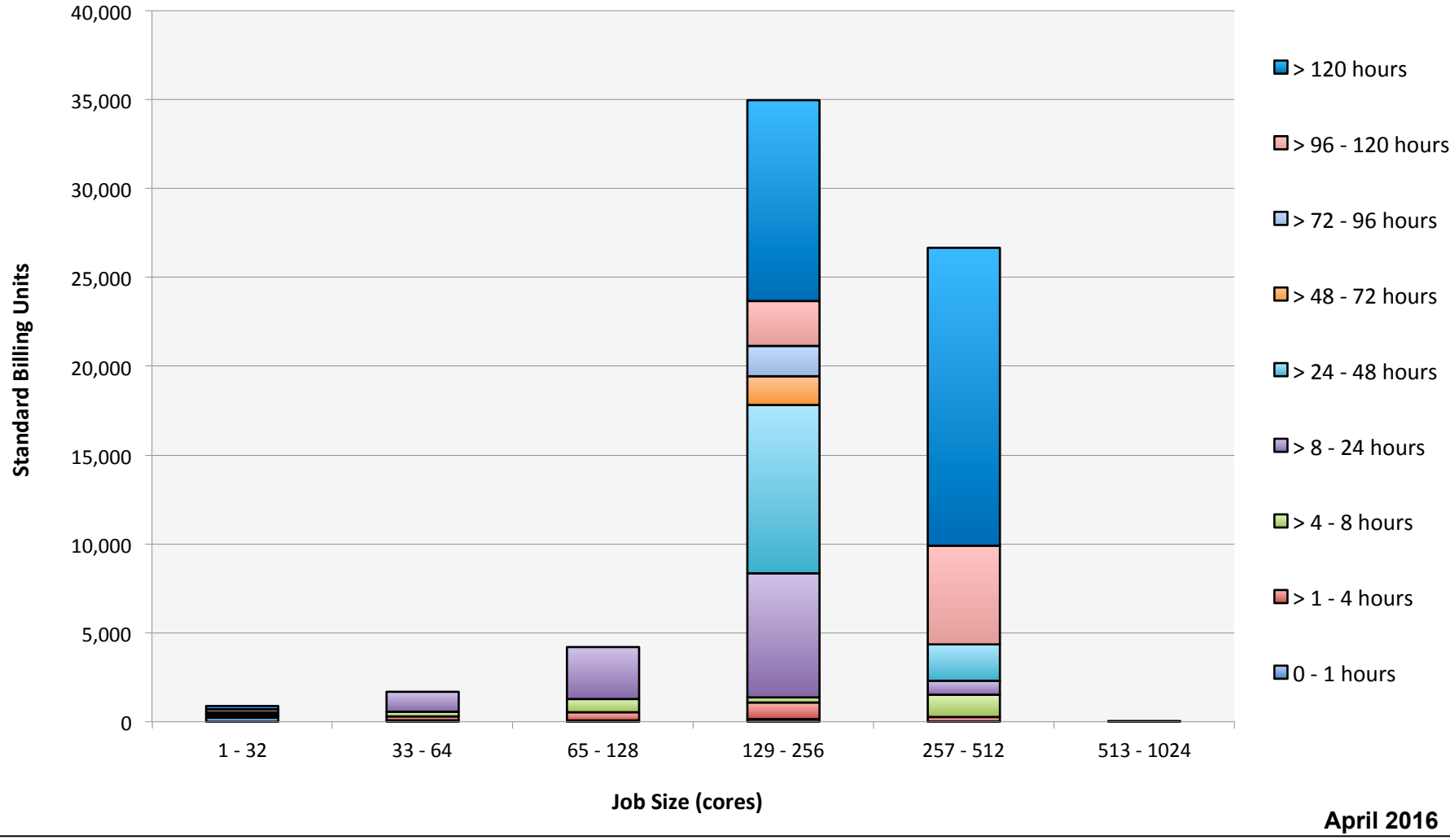
Endeavour:
Monthly Utilization by Job Length



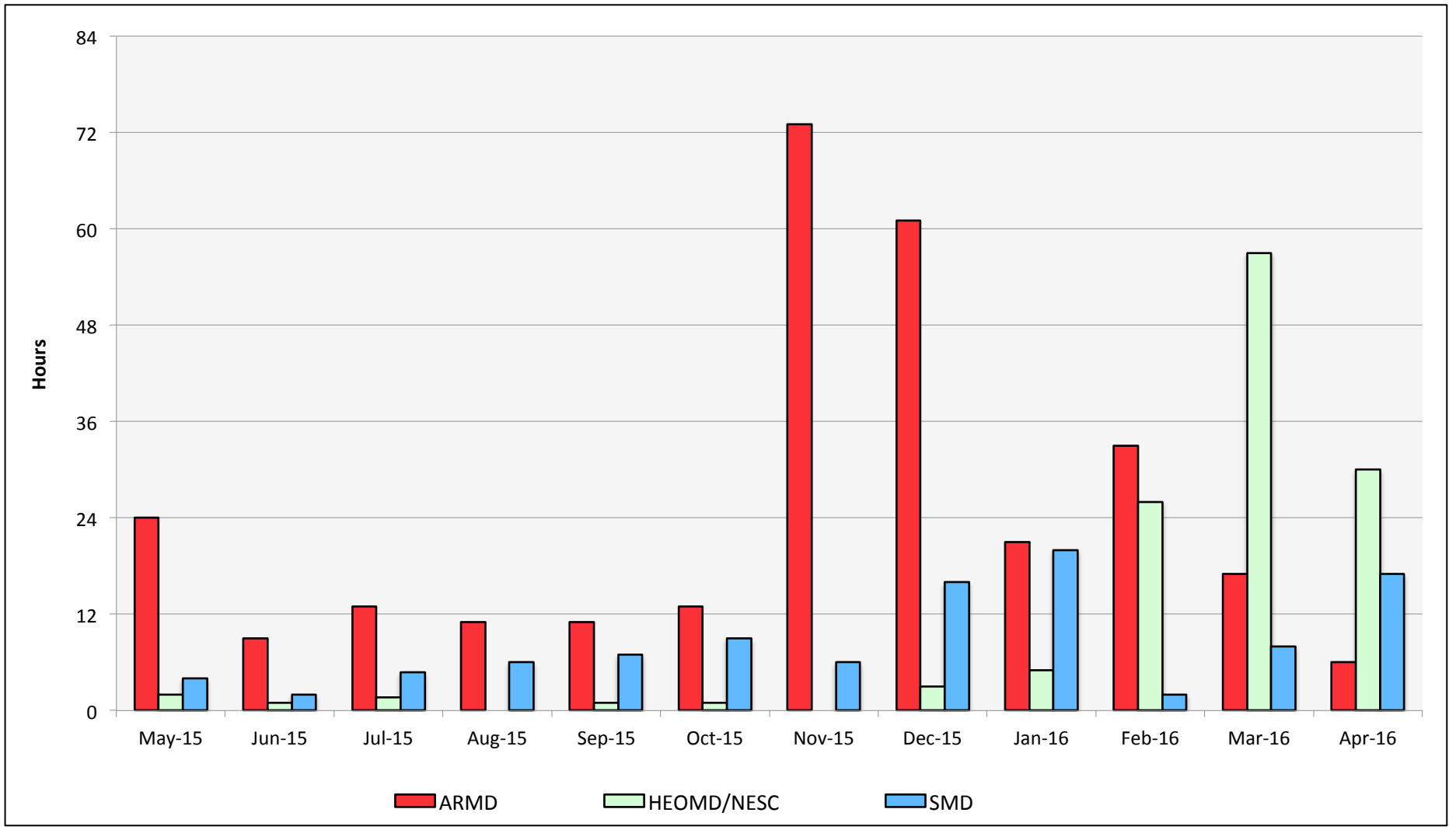
Endeavour:
Monthly Utilization by Size and Mission



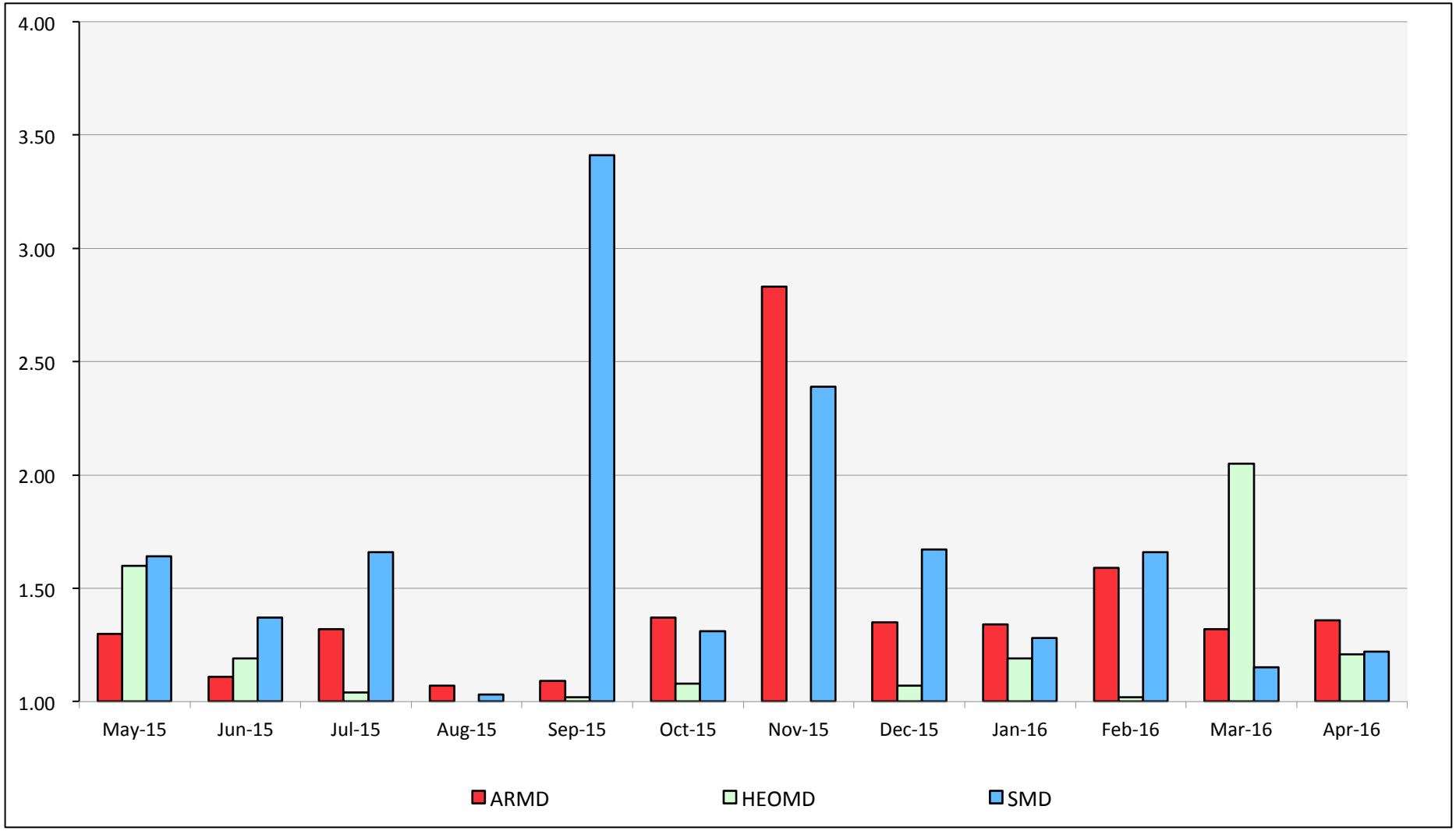
Endeavour:
Monthly Utilization by Size and Length



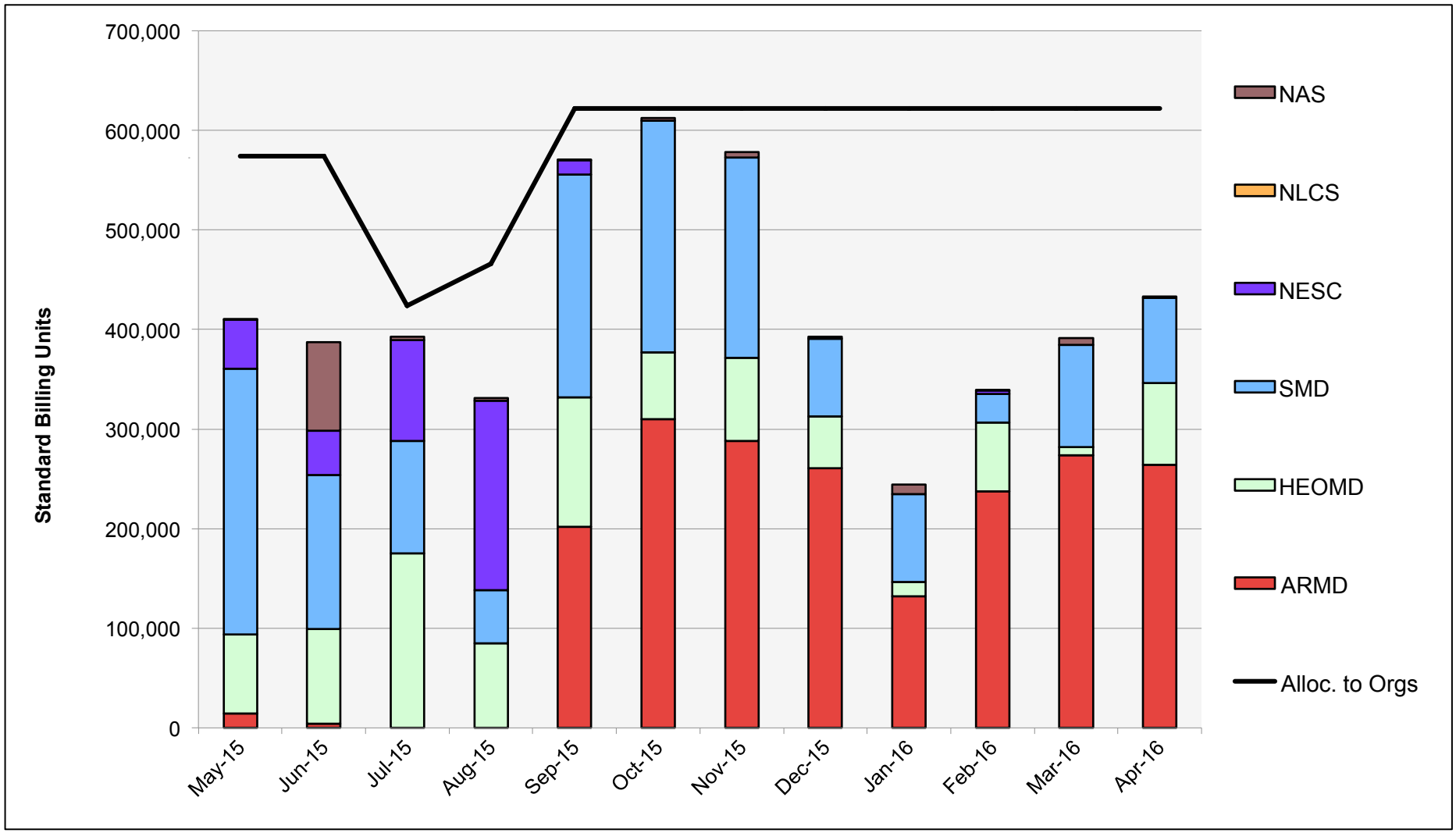
Endeavour:
Average Time to Clear All Jobs



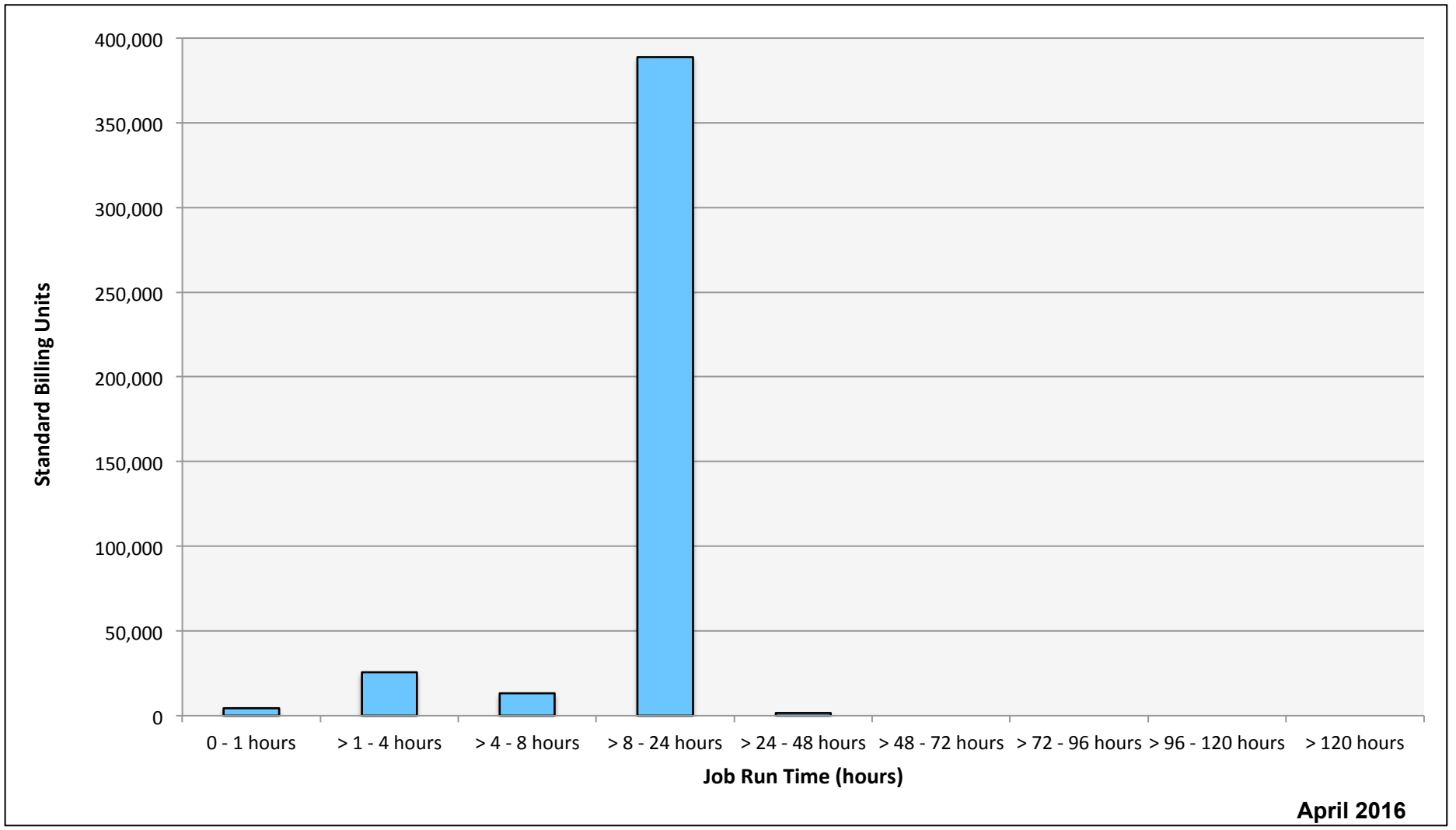
Endeavour:
Average Expansion Factor



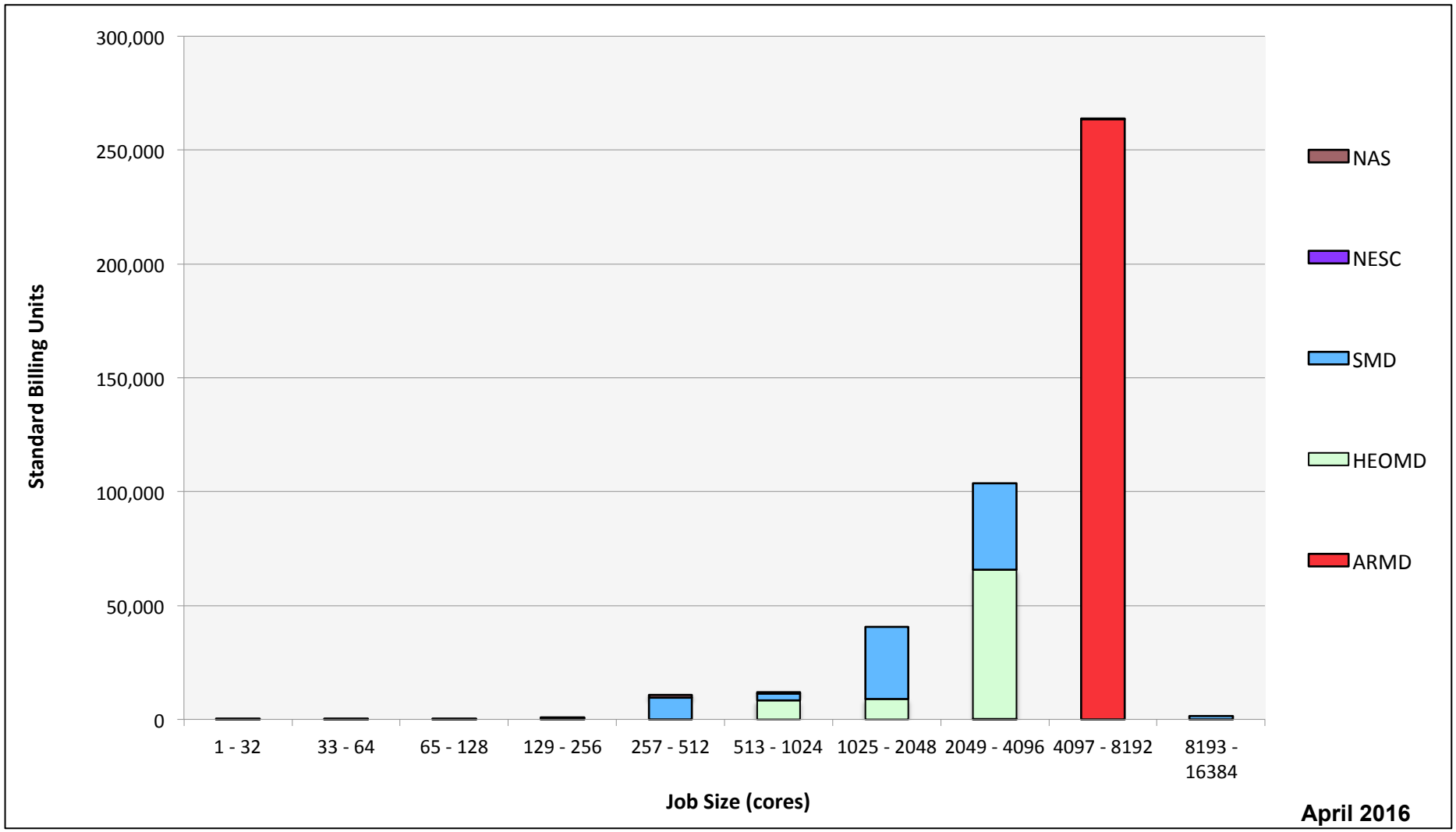
Merope:
SBUs Reported, Normalized to 30-Day Month



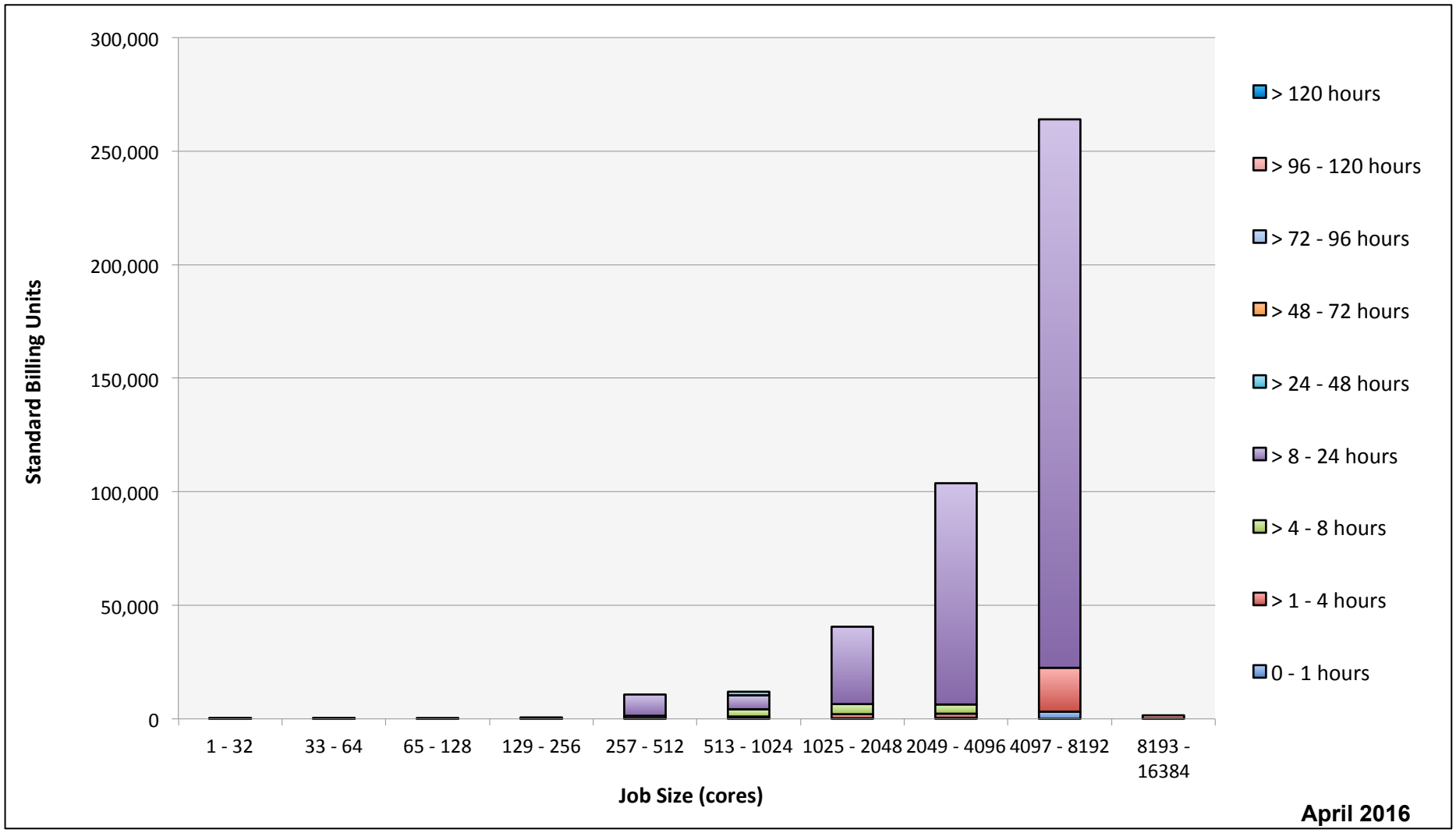
Merope:
Monthly Utilization by Job Length



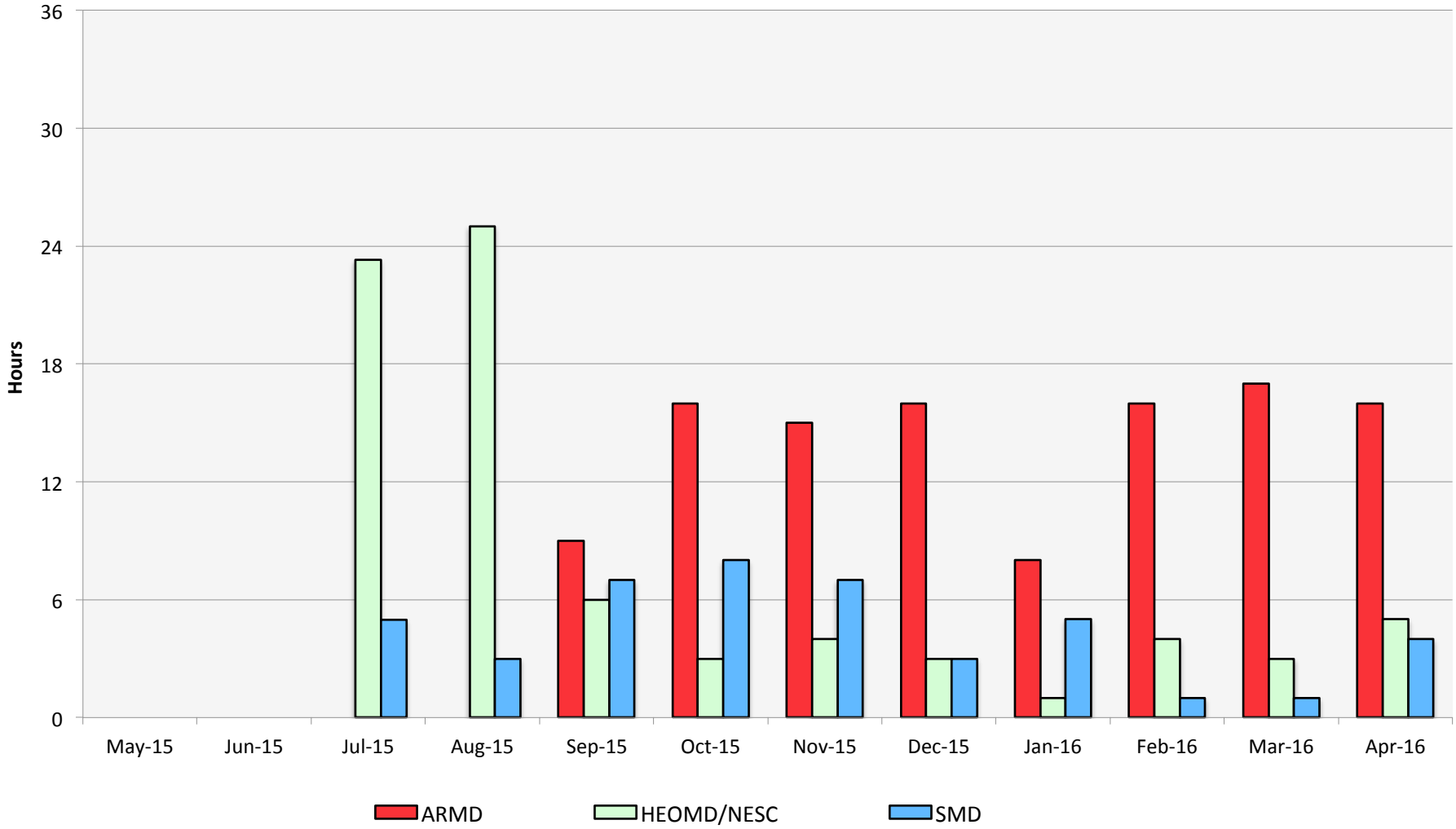
Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Time to Clear All Jobs



Merope:
Average Expansion Factor